

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112421\
 Data File : BM033252.D
 Acq On : 24 Nov 2021 18:12
 Operator : CG/JU
 Sample : M4692-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 WW-EFF

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM033252.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.790	72	77	86	rBV	2674371	3619169	2.05%	0.208%
2	7.054	614	632	638	rBV2	2467774	4601689	2.61%	0.264%
3	8.042	786	800	804	rVV	23428660	68570712	38.83%	3.940%
4	8.125	806	814	823	rVB	1065254	2035213	1.15%	0.117%
5	9.101	971	980	985	rBV	2116977	3498327	1.98%	0.201%
6	9.337	992	1020	1024	rVB	1248289	5811532	3.29%	0.334%
7	10.154	1118	1159	1160	rBV2	1358743	7094638	4.02%	0.408%
8	12.142	1490	1497	1503	rBV	2487597	3610451	2.04%	0.207%
9	12.960	1614	1636	1641	rBV	3744245	13852178	7.85%	0.796%
10	13.077	1650	1656	1663	rVV	1655280	2475026	1.40%	0.142%
11	13.183	1667	1674	1685	rVV	4522912	6918073	3.92%	0.397%
12	13.377	1699	1707	1710	rBV	1720106	2464547	1.40%	0.142%
13	13.442	1710	1718	1725	rVV	2757264	5769350	3.27%	0.331%
14	13.519	1725	1731	1745	rVB	3950852	6231246	3.53%	0.358%
15	13.707	1758	1763	1769	rVB	2571396	3707281	2.10%	0.213%
16	13.772	1769	1774	1779	rBV	7451199	9801890	5.55%	0.563%
17	14.224	1842	1851	1858	rBV	29107841	58255772	32.99%	3.347%
18	14.448	1884	1889	1891	rBV	2304143	3152566	1.79%	0.181%
19	14.501	1895	1898	1903	rVB	1615845	1985131	1.12%	0.114%
20	14.577	1903	1911	1912	rBV2	1869839	3333787	1.89%	0.192%
21	14.754	1935	1941	1945	rBV	1838841	2718838	1.54%	0.156%
22	14.807	1945	1950	1955	rVV	4789685	6290588	3.56%	0.361%
23	15.213	1982	2019	2022	rBV	32065266	176569565	100.00%	10.145%
24	15.554	2074	2077	2083	rVB	1477277	1978234	1.12%	0.114%
25	15.742	2104	2109	2115	rVV	2440303	3467809	1.96%	0.199%
26	16.048	2158	2161	2165	rVV2	2639646	3771481	2.14%	0.217%
27	16.101	2165	2170	2182	rVB	14012372	24400395	13.82%	1.402%
28	16.489	2221	2236	2237	rBV2	29150254	64525452	36.54%	3.707%
29	16.613	2252	2257	2261	rVB2	32185702	69136739	39.16%	3.972%
30	16.754	2269	2281	2284	rBV2	11866129	30988039	17.55%	1.780%
31	16.789	2284	2287	2300	rVB2	6356495	15418604	8.73%	0.886%
32	16.918	2304	2309	2316	rBV	9840753	13074262	7.40%	0.751%
33	17.024	2323	2327	2330	rVV	1583027	2385376	1.35%	0.137%
34	17.060	2330	2333	2340	rVB2	2513309	4202926	2.38%	0.241%
35	17.301	2370	2374	2381	rVB	1193546	1856734	1.05%	0.107%
36	18.224	2519	2531	2535	rBV	16784524	40717832	23.06%	2.339%

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Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	18.265	2535	2538	2543	rVB	2392619	3111816	1.76%	0.179%
38	18.418	2560	2564	2569	rVV	7683671	9422871	5.34%	0.541%
39	18.483	2570	2575	2586	rVB	1809332	3549093	2.01%	0.204%
40	18.606	2591	2596	2600	rVB	2732290	3421337	1.94%	0.197%
41	18.948	2650	2654	2656	rBV	1481857	1950542	1.10%	0.112%
42	18.977	2656	2659	2663	rVB	2991519	3549685	2.01%	0.204%
43	19.048	2668	2671	2675	rVB	2639414	2980443	1.69%	0.171%
44	19.124	2676	2684	2689	rBV2	6155098	10797107	6.11%	0.620%
45	19.236	2700	2703	2704	rBV	2232750	2246883	1.27%	0.129%
46	19.259	2704	2707	2711	rVB	3033487	3411727	1.93%	0.196%
47	19.383	2714	2728	2731	rBV2	15909005	41407853	23.45%	2.379%
48	19.430	2731	2736	2742	rVV3	11711990	24216513	13.71%	1.391%
49	19.518	2742	2751	2757	rVV4	30530671	73428104	41.59%	4.219%
50	19.653	2767	2774	2777	rBV2	24152367	40511075	22.94%	2.327%
51	19.677	2777	2778	2781	rVV	10857443	10084228	5.71%	0.579%
52	19.706	2781	2783	2793	rVB2	3374264	4384490	2.48%	0.252%
53	19.818	2793	2802	2807	rBV2	34240881	72375284	40.99%	4.158%
54	19.912	2813	2818	2823	rVB	4576573	5985359	3.39%	0.344%
55	19.965	2823	2827	2831	rBV	7672442	8813058	4.99%	0.506%
56	20.059	2838	2843	2847	rVB2	2513299	3987200	2.26%	0.229%
57	20.106	2847	2851	2856	rVB	2064868	2561678	1.45%	0.147%
58	20.177	2859	2863	2866	rBV	2283322	2607564	1.48%	0.150%
59	20.283	2874	2881	2887	rBV	4299420	9311046	5.27%	0.535%
60	20.365	2888	2895	2899	rVB	33778222	62026146	35.13%	3.564%
61	20.418	2899	2904	2907	rBV2	1169084	2488992	1.41%	0.143%
62	20.459	2908	2911	2914	rBV3	2638968	3561880	2.02%	0.205%
63	20.500	2914	2918	2921	rVB	5603530	6419167	3.64%	0.369%
64	20.642	2921	2942	2947	rBV4	27430767	144829727	82.02%	8.321%
65	20.777	2962	2965	2974	rVB	2572637	5464862	3.10%	0.314%
66	20.877	2975	2982	2986	rBV	32751733	56389827	31.94%	3.240%
67	20.918	2986	2989	2993	rVB	2565882	3519650	1.99%	0.202%
68	20.995	2993	3002	3006	rBV	7167159	14592270	8.26%	0.838%
69	21.177	3028	3033	3037	rVB	15676501	19184402	10.87%	1.102%
70	21.347	3056	3062	3066	rBV	30191644	44307570	25.09%	2.546%
71	21.418	3071	3074	3078	rVB	1997442	2483329	1.41%	0.143%
72	22.006	3169	3174	3179	rBV2	11169509	22421437	12.70%	1.288%
73	22.077	3179	3186	3191	rVB2	31857663	70798080	40.10%	4.068%
74	22.383	3235	3238	3243	rVB	1403351	1800842	1.02%	0.103%
75	23.042	3343	3350	3355	rBV	9820140	22205991	12.58%	1.276%
76	23.159	3359	3370	3372	rBV3	27961547	84543497	47.88%	4.857%

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Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	23.483	3420	3425	3431	rVB	3121766	5024665	2.85%	0.289%
78	24.441	3583	3588	3595	rVB	1813456	3436302	1.95%	0.197%
79	25.024	3681	3687	3696	rVB	3998289	9222520	5.22%	0.530%
80	26.835	3987	3995	4000	rBV2	2578544	7914271	4.48%	0.455%
81	28.165	4192	4221	4222	rBV2	18458939	120926009	68.49%	6.948%
82	29.371	4419	4426	4429	rBV2	1911050	4573664	2.59%	0.263%

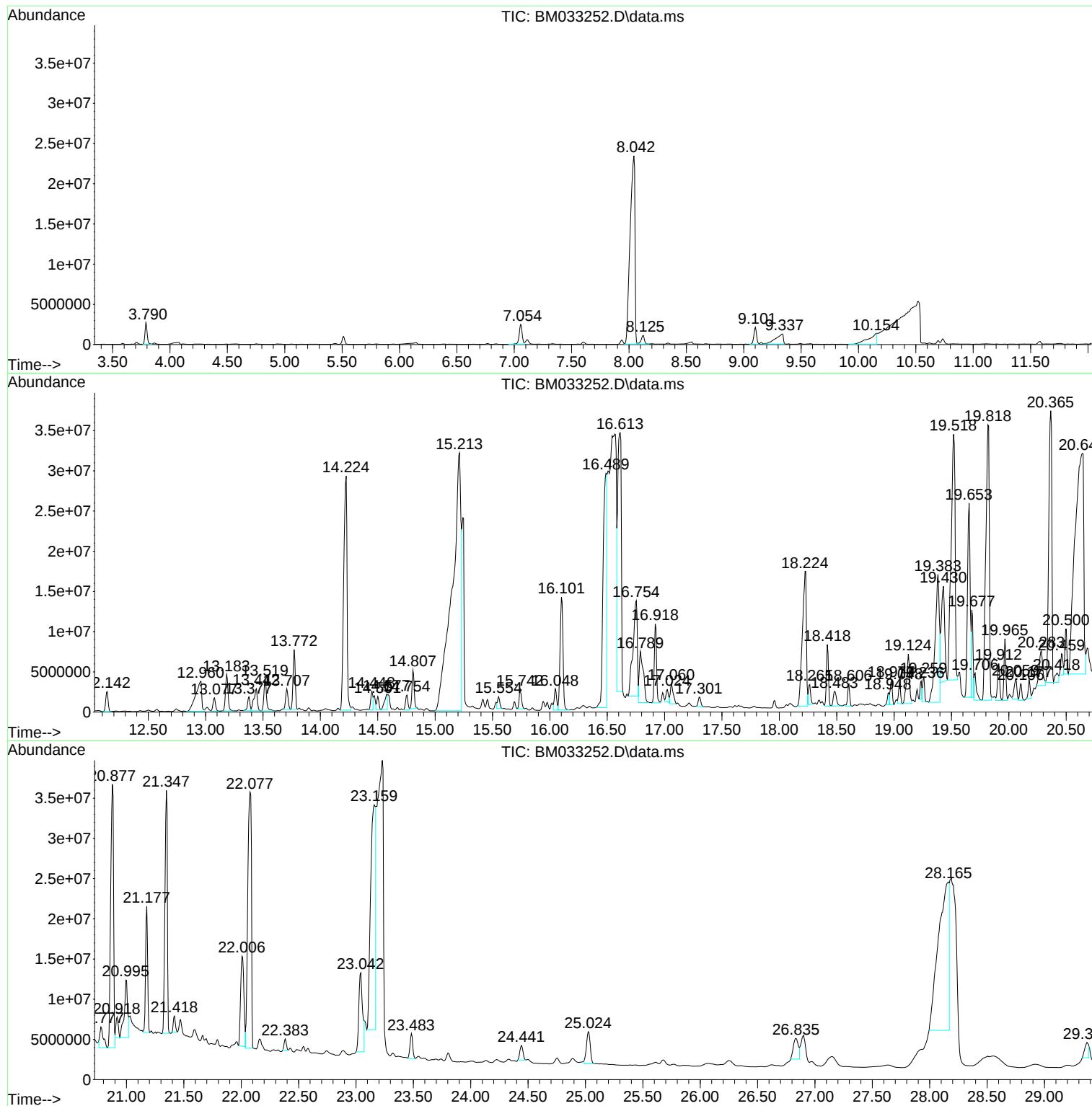
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112421\
Data File : BM033252.D
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Operator : CG/JU
Sample : M4692-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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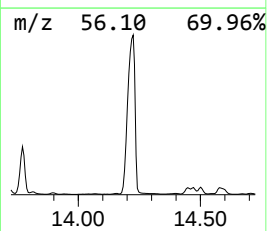
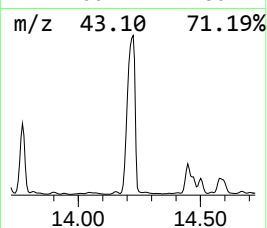
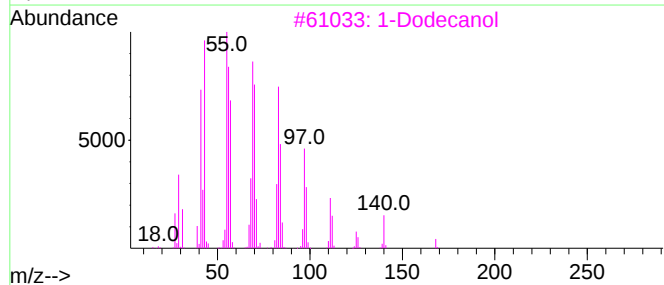
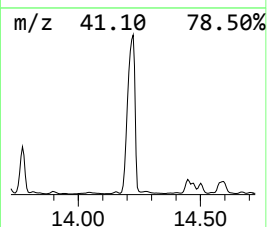
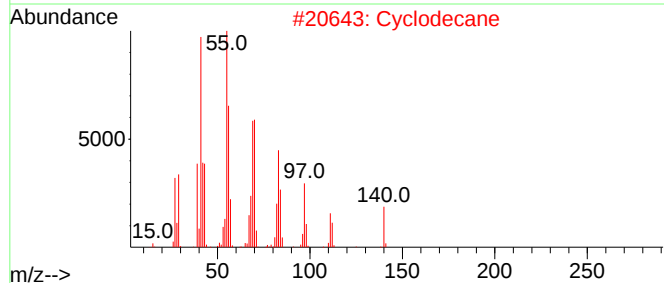
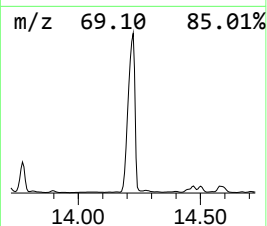
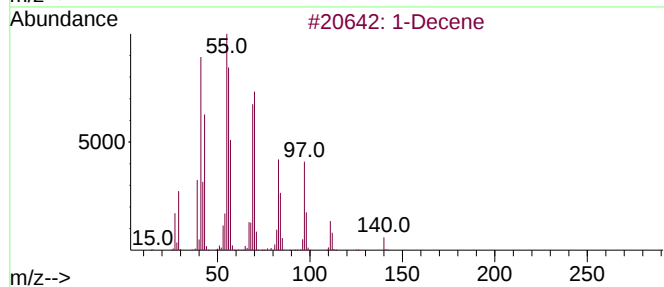
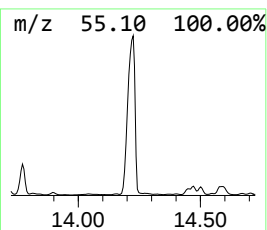
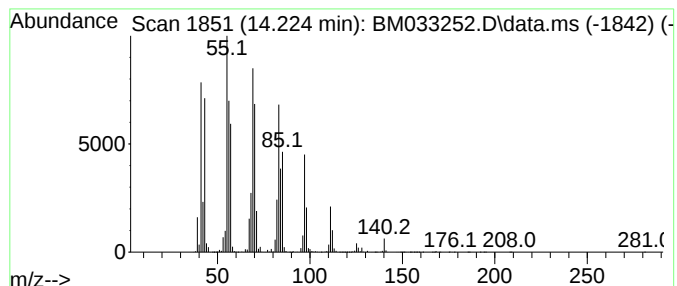
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 1-Decene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.224	349.49 ng	58255800	Acenaphthene-d10	14.560

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decene		140	C10H20	000872-05-9	93
2	Cyclodecane		140	C10H20	000293-96-9	93
3	1-Dodecanol		186	C12H26O	000112-53-8	90
4	Cetene		224	C16H32	000629-73-2	86
5	3-Chloropropionic acid, dodecyl ...		276	C15H29ClO2	074316-16-8	86



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ALS Vial : 13 Sample Multiplier: 1

Instrument :
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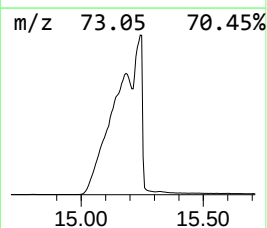
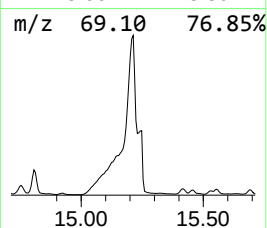
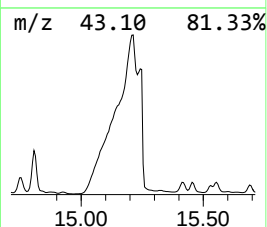
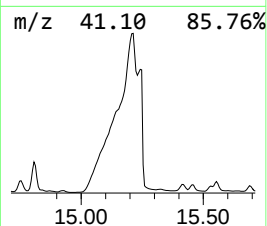
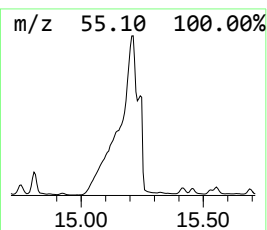
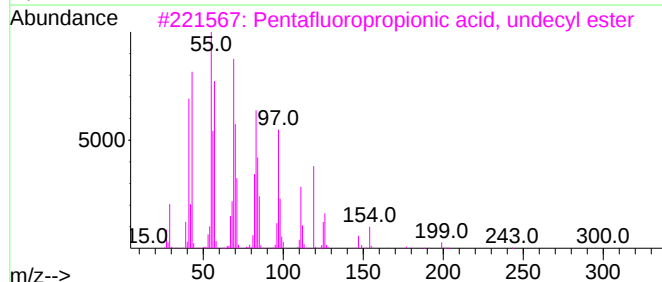
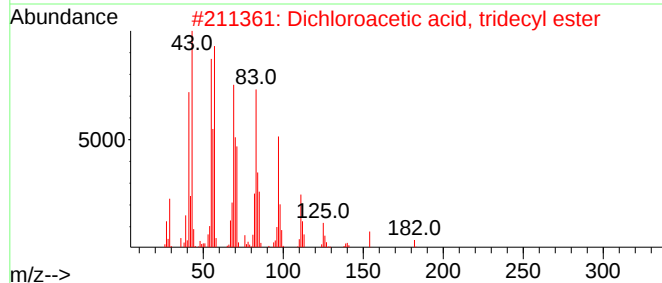
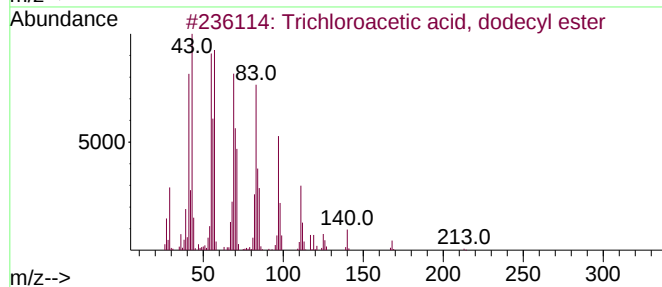
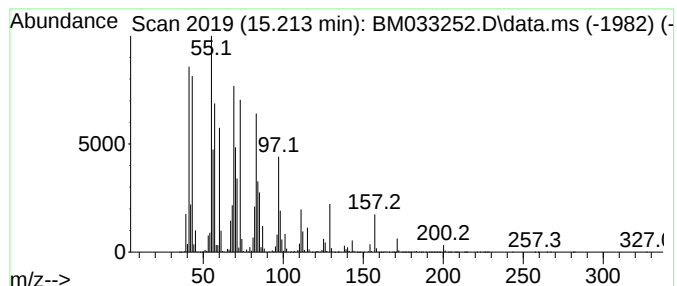
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Trichloroacetic acid, dodec... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.213	1059.27 ng	176570000	Acenaphthene-d10	14.560

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, dodecyl ester	330	C14H25Cl3O2	074339-50-7	90
2			Dichloroacetic acid, tridecyl ester	310	C15H28Cl2O2	1000280-48-3	90
3			Pentafluoropropionic acid, undec...	318	C14H23F5O2	959014-11-0	81
4			9-Octadecene, (E)-	252	C18H36	007206-25-9	76
5			1-Tetradecanol	214	C14H30O	000112-72-1	74



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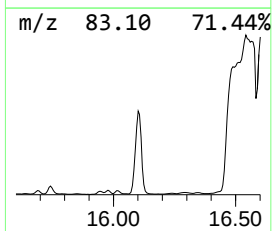
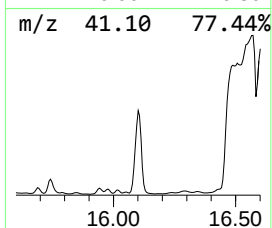
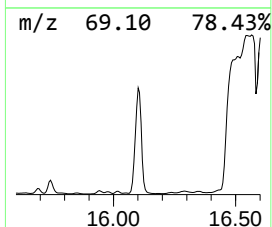
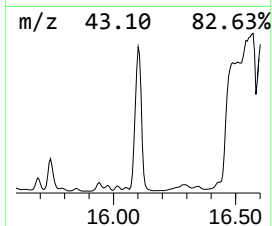
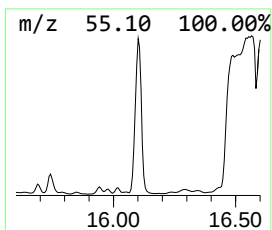
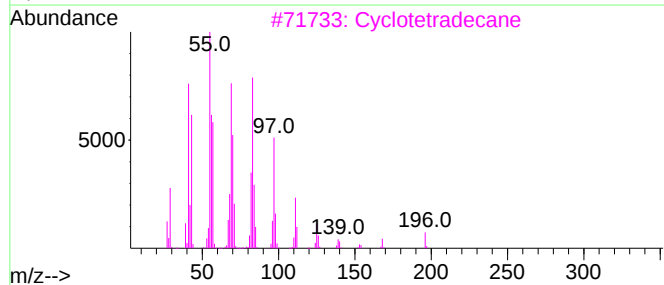
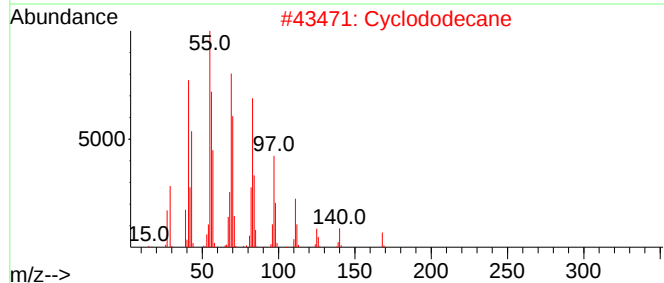
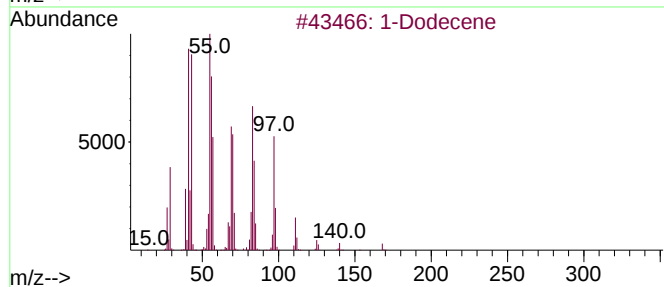
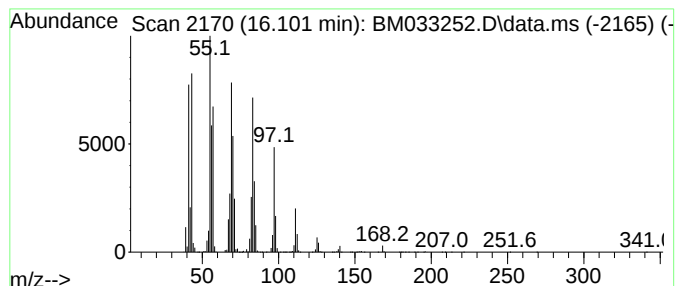
Instrument :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Dodecene Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.101	262.83 ng	24400400	Phenanthrene-d10	17.307
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1	1-Dodecene	168 C12H24	000112-41-4	96
2	Cyclododecane	168 C12H24	000294-62-2	95
3	Cyclotetradecane	196 C14H28	000295-17-0	93
4	1-Tetradecanol	214 C14H30O	000112-72-1	91
5	1-Hexadecanol	242 C16H34O	036653-82-4	91



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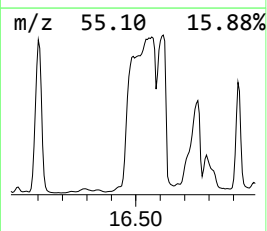
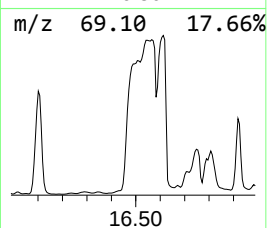
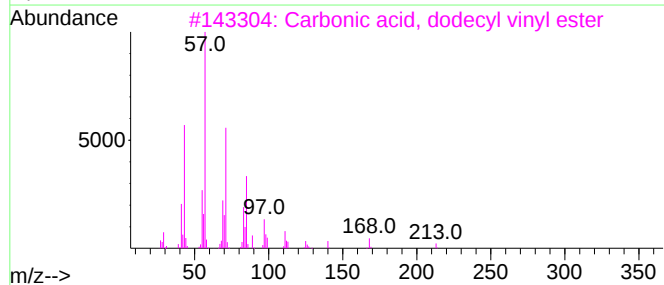
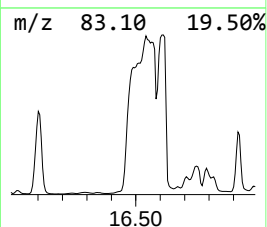
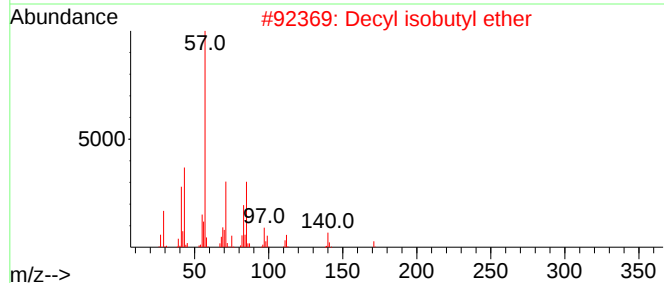
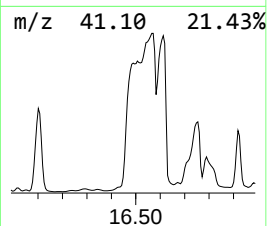
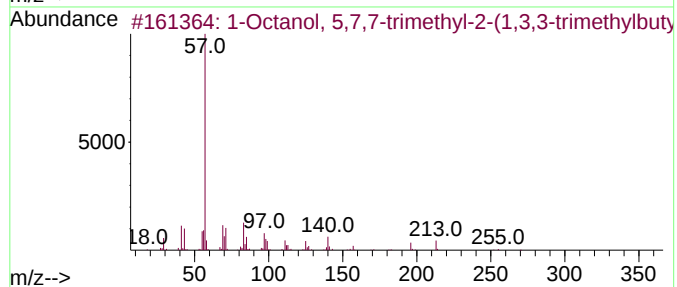
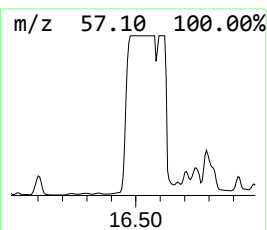
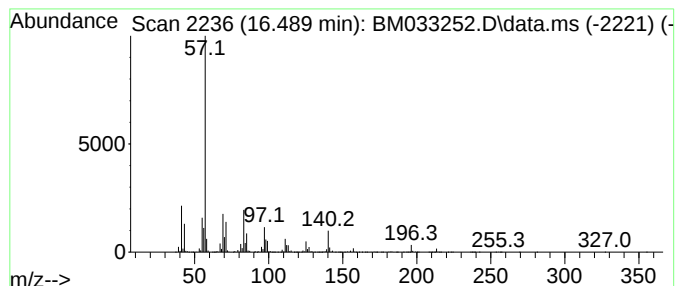
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Octanol, 5,7,7-trimethyl-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.489	695.04 ng	64525500	Phenanthrene-d10	17.307

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Octanol, 5,7,7-trimethyl-2-(1,...	270	C18H38O	036400-98-3	80
2		Decyl isobutyl ether	214	C14H30O	1010406-32-5	64
3		Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	64
4		Hexanoic acid, 3,5,5-trimethyl-,...	340	C22H44O2	1000406-26-2	59
5		Butyl octadecyl ether	326	C22H46O	1000406-40-6	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112421\
Data File : BM033252.D
Acq On : 24 Nov 2021 18:12
Operator : CG/JU
Sample : M4692-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WW-EFF

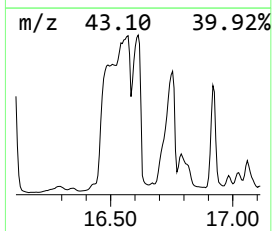
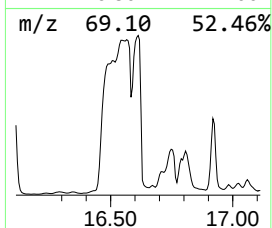
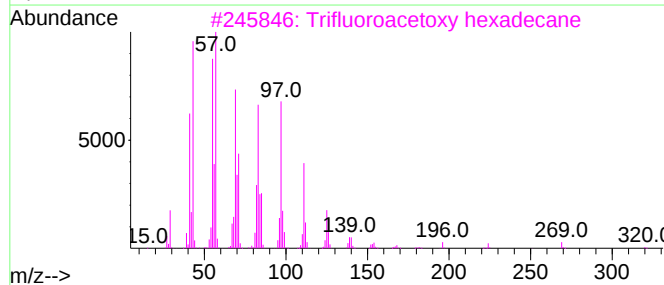
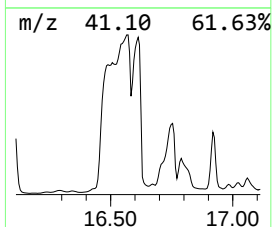
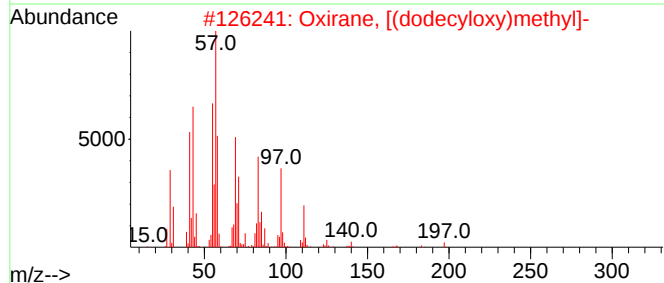
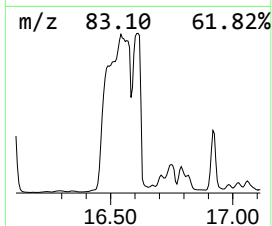
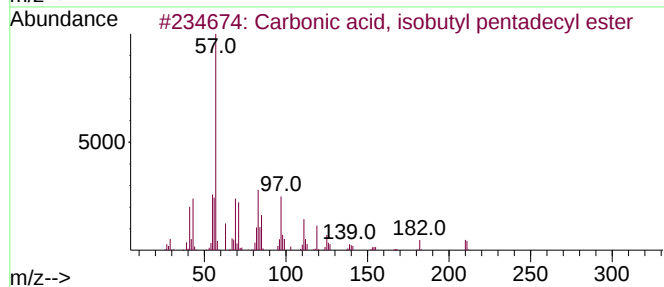
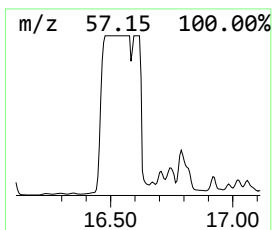
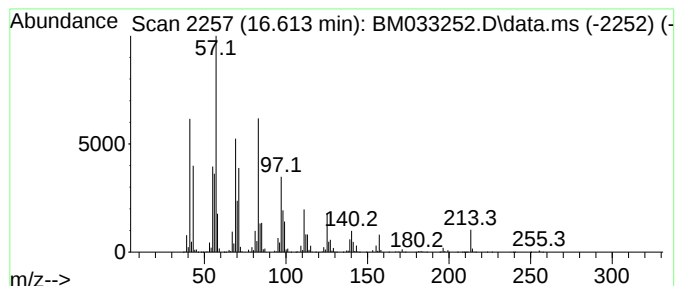
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Carbonic acid, isobutyl pen... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.613	744.71 ng	69136700	Phenanthrene-d10	17.307

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, isobutyl pentadec...	328	C20H40O3	1000314-61-2	53
2			Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	47
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	43
4			1-Nonadecene	266	C19H38	018435-45-5	38
5			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112421\
Data File : BM033252.D
Acq On : 24 Nov 2021 18:12
Operator : CG/JU
Sample : M4692-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WW-EFF

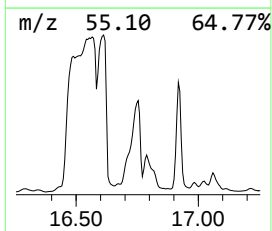
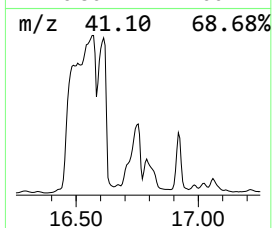
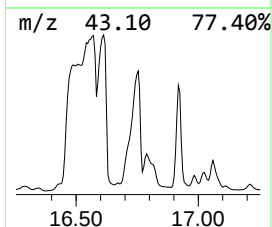
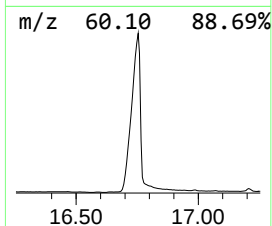
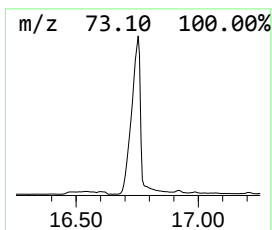
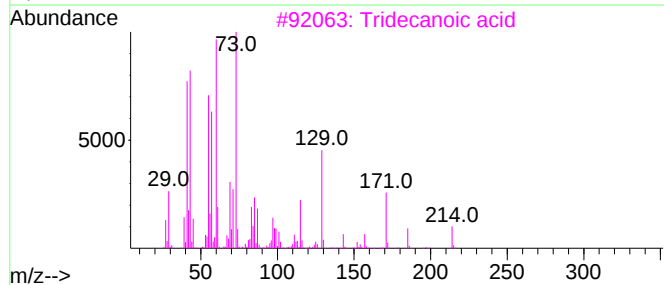
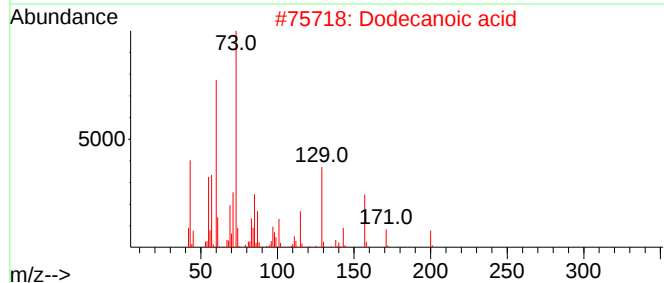
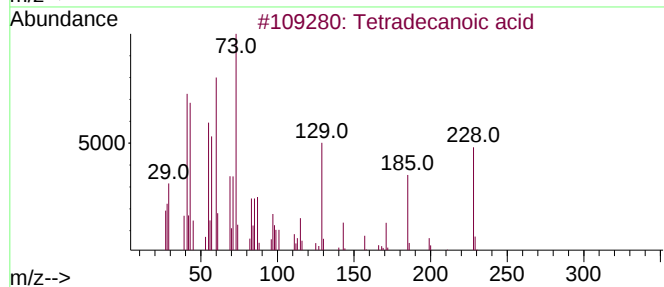
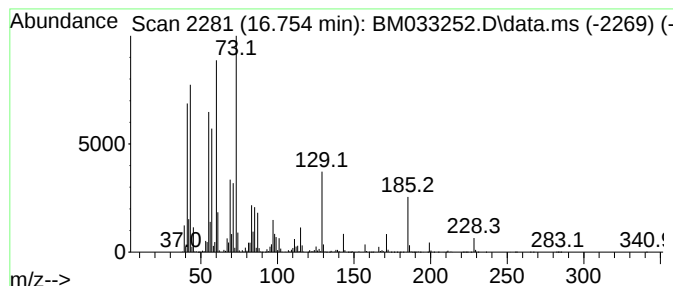
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Tetradecanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.754	333.79 ng	30988000	Phenanthrene-d10	17.307

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
2			Dodecanoic acid	200	C12H24O2	000143-07-7	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	86
4			Undecanoic acid	186	C11H22O2	000112-37-8	52
5			n-Decanoic acid	172	C10H20O2	000334-48-5	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112421\
Data File : BM033252.D
Acq On : 24 Nov 2021 18:12
Operator : CG/JU
Sample : M4692-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WW-EFF

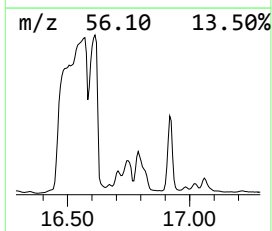
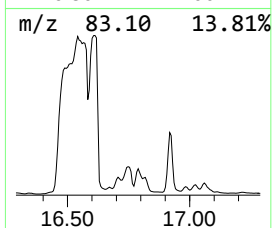
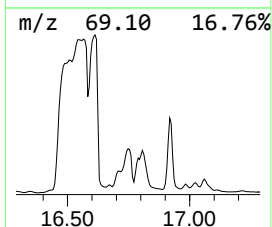
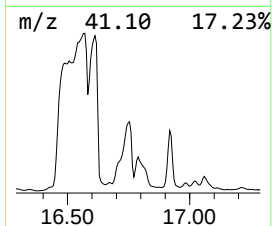
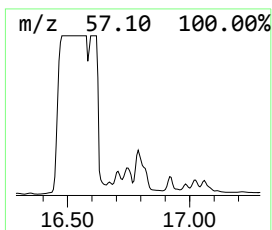
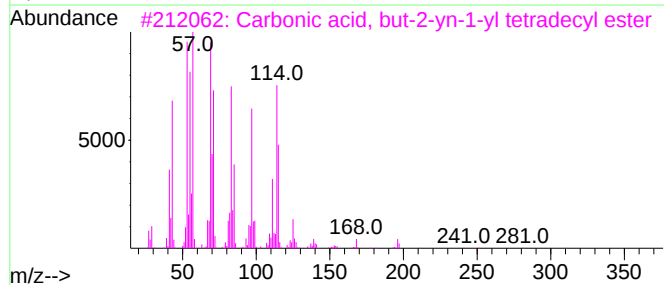
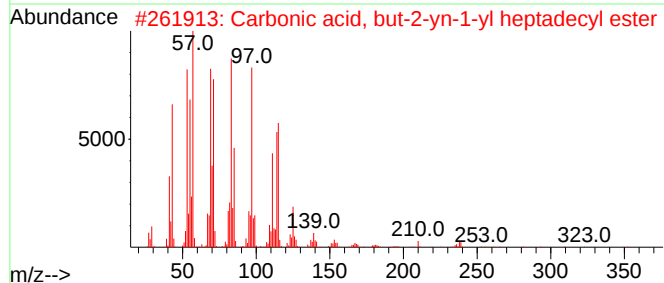
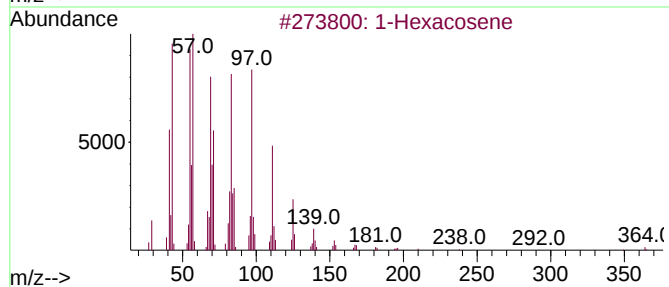
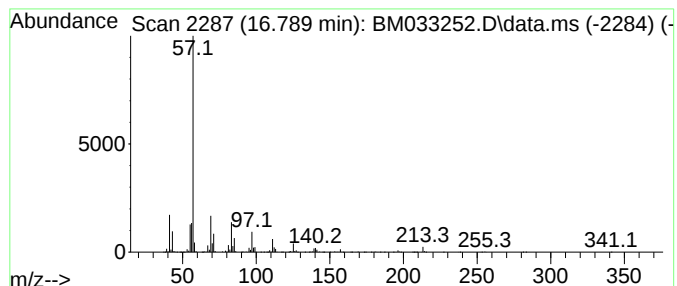
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1-Hexacosene Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.789	166.08 ng	15418600	Phenanthrene-d10	17.307

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene			364	C26H52	018835-33-1	53
2	Carbonic acid, but-2-yn-1-yl hep...			352	C22H40O3	1000383-21-2	53
3	Carbonic acid, but-2-yn-1-yl tet...			310	C19H34O3	1010383-20-9	50
4	Methyl tetratriacontyl ether			509	C35H72O	1000406-30-1	47
5	Dotriacontyl pentafluoropropionate			612	C35H65F5O2	1010351-81-4	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112421\
Data File : BM033252.D
Acq On : 24 Nov 2021 18:12
Operator : CG/JU
Sample : M4692-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

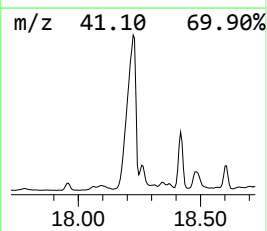
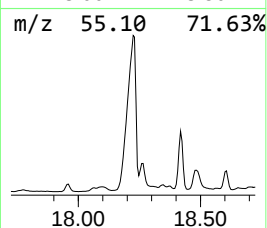
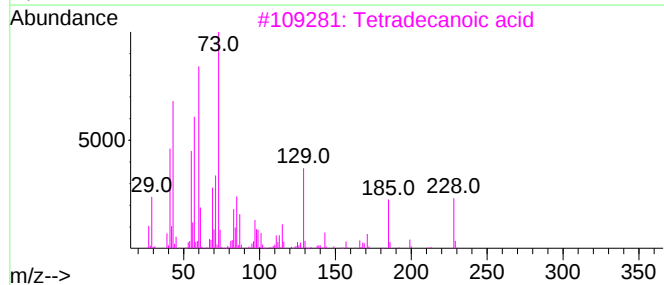
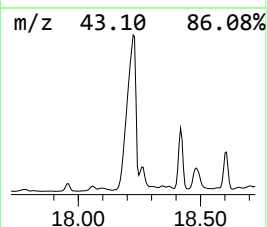
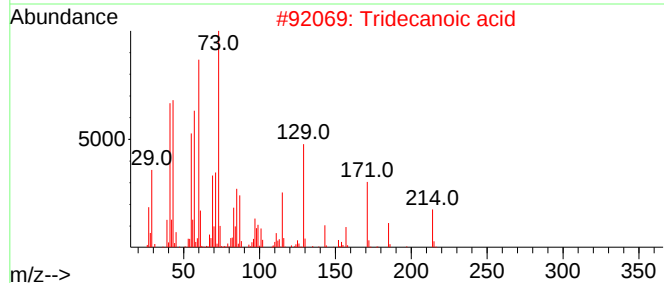
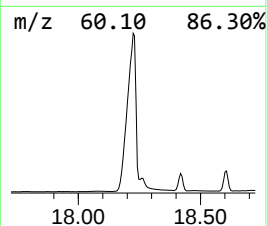
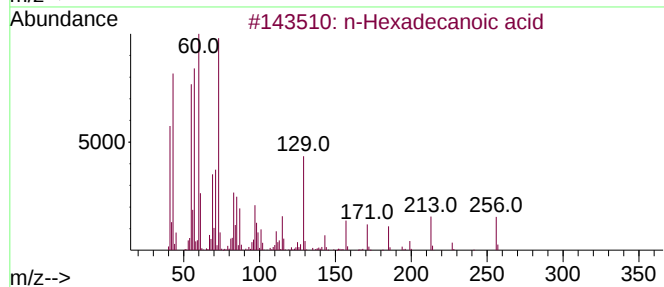
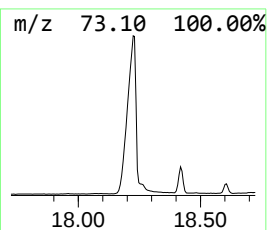
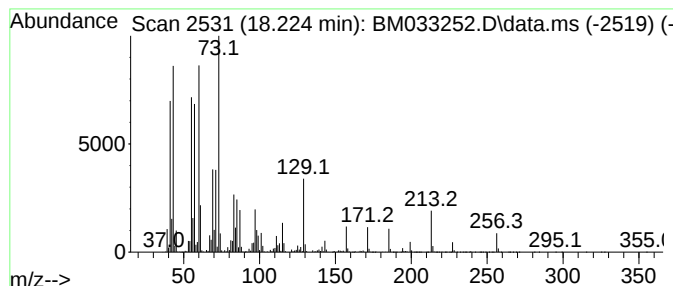
Instrument :
BNA_M
ClientSampleId :
WW-EFF

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.224	438.60 ng	40717800	Phenanthrene-d10	17.307	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112421\
Data File : BM033252.D
Acq On : 24 Nov 2021 18:12
Operator : CG/JU
Sample : M4692-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WW-EFF

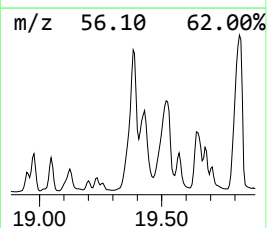
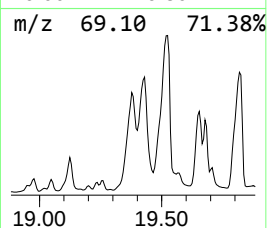
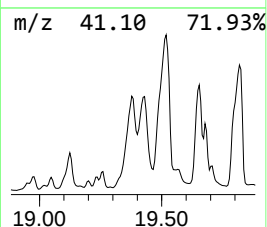
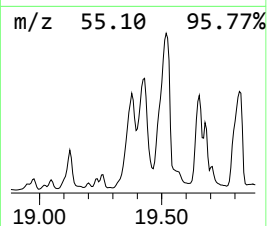
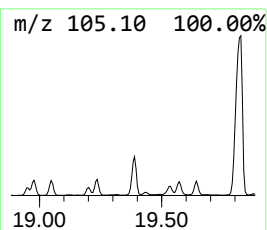
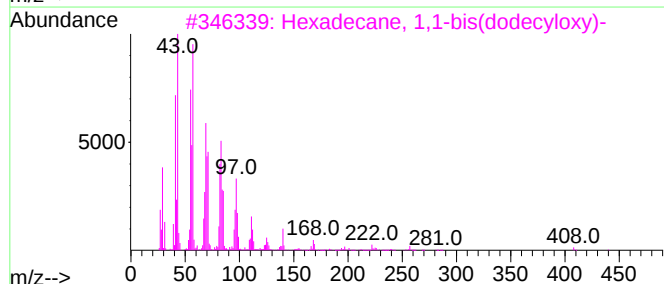
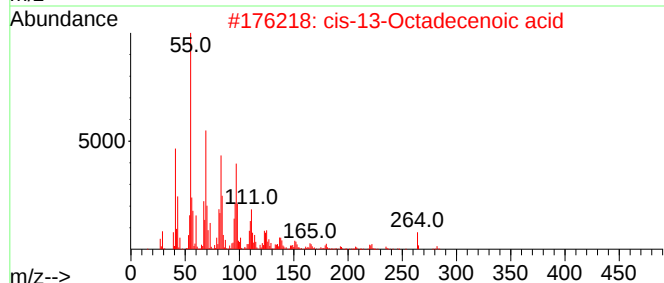
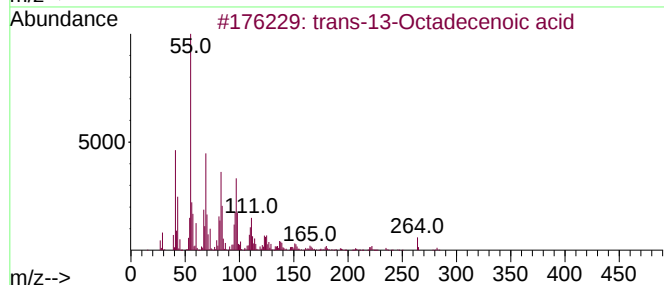
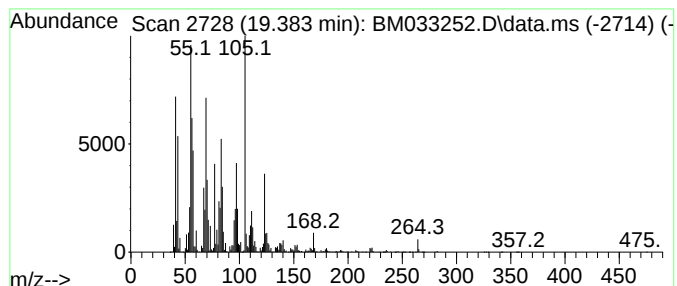
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 trans-13-Octadecenoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.383	446.03 ng	41407900	Phenanthrene-d10	17.307

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	96
2			cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	91
3			Hexadecane, 1,1-bis(dodecyloxy)-	595	C40H82O2	056554-64-4	68
4			Pentadecafluorooctanoic acid, do...	582	C20H25F15O2	1000406-04-2	62
5			Chloroacetic acid, dodecyl ester	262	C14H27ClO2	006316-04-7	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112421\
Data File : BM033252.D
Acq On : 24 Nov 2021 18:12
Operator : CG/JU
Sample : M4692-01
Misc :
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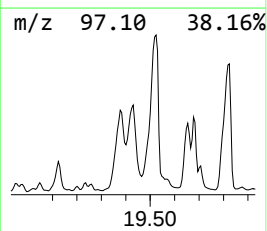
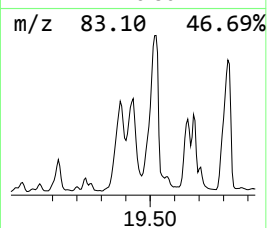
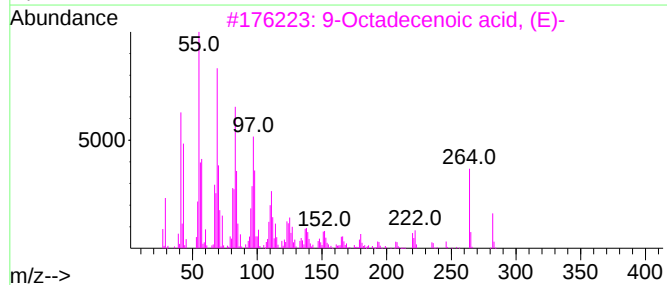
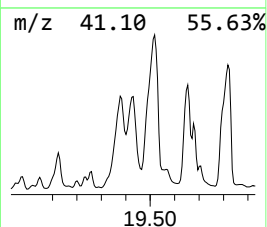
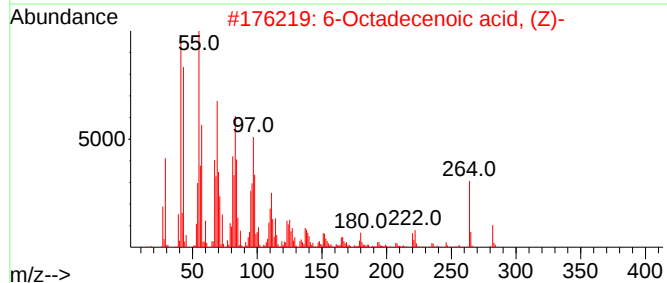
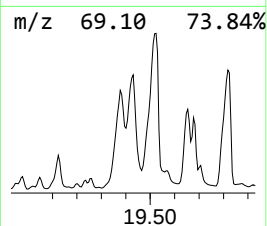
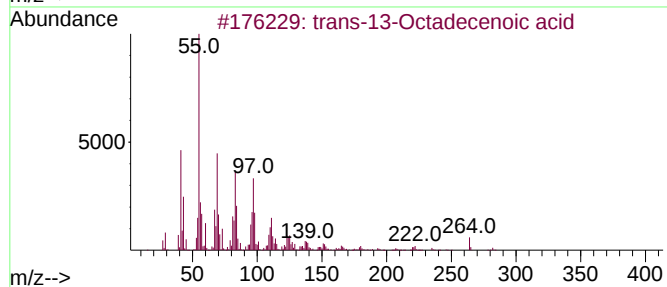
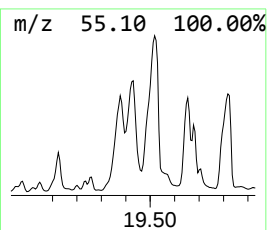
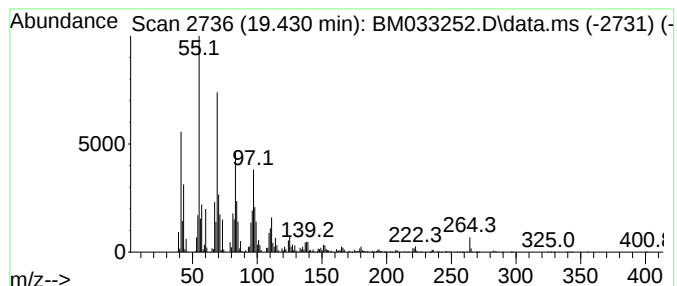
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 6-Octadecenoic acid, (Z)- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.430	195.03 ng	24216500	Chrysene-d12	21.465	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	89
2	6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	89
3	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	87
4	6-Tetradecene, (Z)-	196	C14H28	041446-61-1	74
5	Acetic acid, trifluoro-, nonyl e...	240	C11H19F3O2	030767-14-7	64



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Acq On : 24 Nov 2021 18:12
Operator : CG/JU
Sample : M4692-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WW-EFF

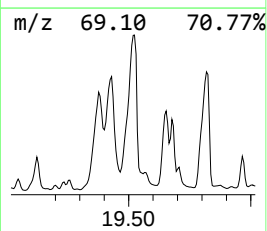
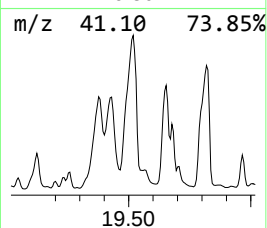
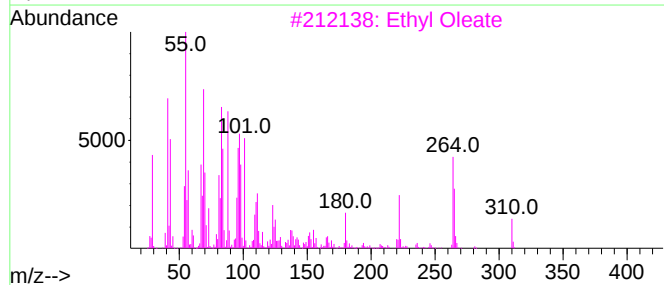
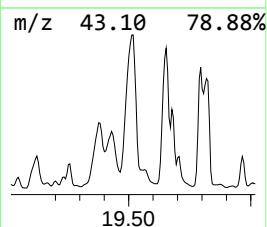
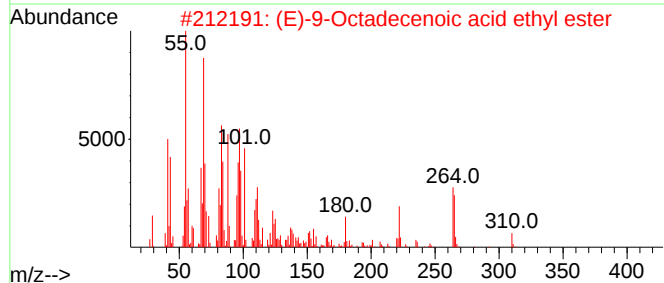
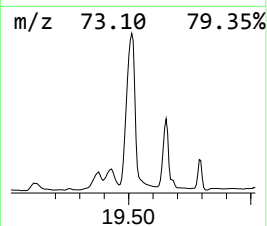
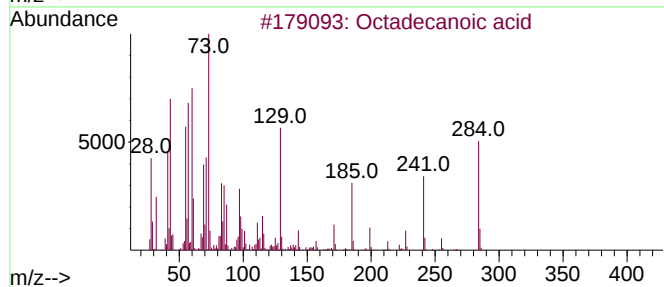
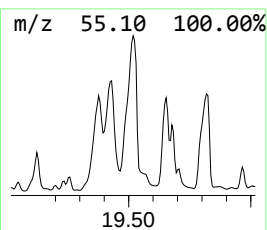
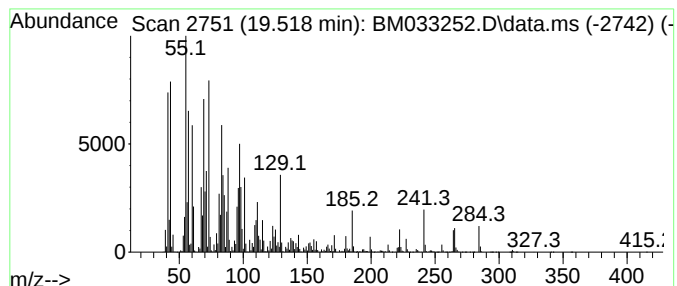
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.518	591.37 ng	73428100	Chrysene-d12	21.465

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	96
2			(E)-9-Octadecenoic acid ethyl ester	310	C20H38O2	006114-18-7	95
3			Ethyl Oleate	310	C20H38O2	000111-62-6	95
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5			Oleic Acid	282	C18H34O2	000112-80-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112421\
Data File : BM033252.D
Acq On : 24 Nov 2021 18:12
Operator : CG/JU
Sample : M4692-01
Misc :
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ClientSampleId :
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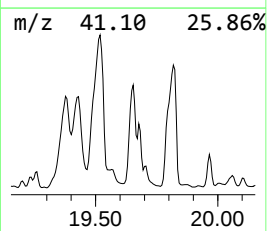
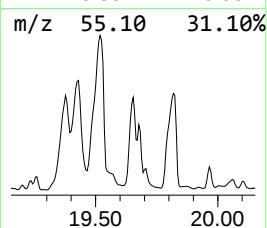
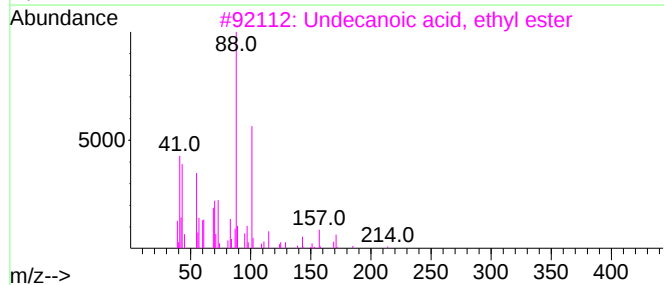
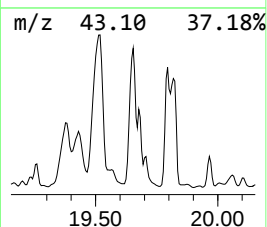
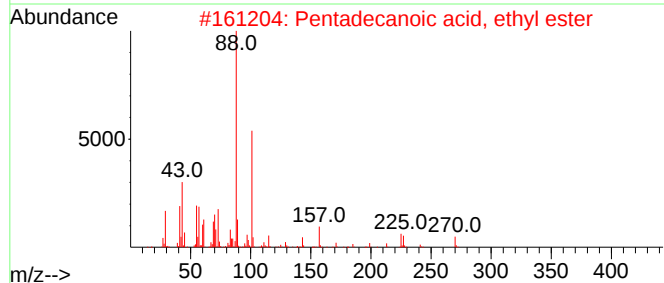
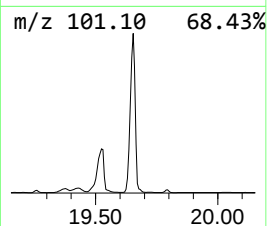
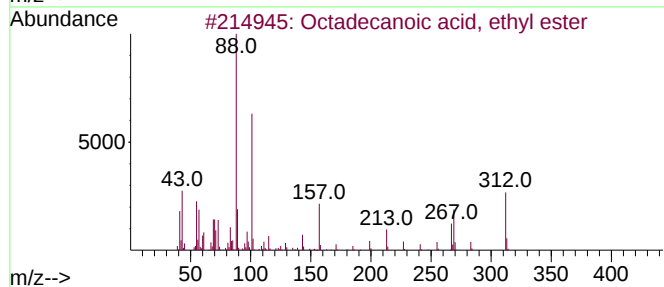
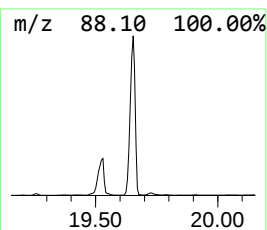
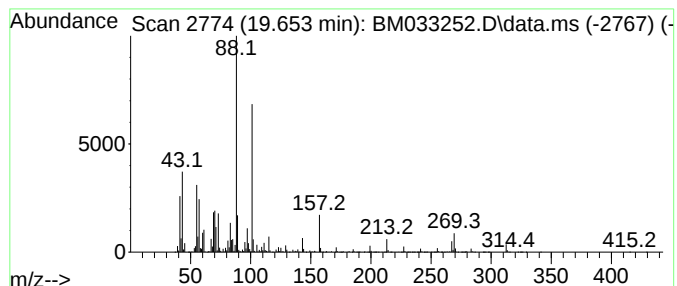
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Octadecanoic acid, ethyl ester Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.654	326.26 ng	40511100	Chrysene-d12	21.465

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid, ethyl ester	312	C20H40O2	000111-61-5	99
2		Pentadecanoic acid, ethyl ester	270	C17H34O2	041114-00-5	94
3		Undecanoic acid, ethyl ester	214	C13H26O2	000627-90-7	91
4		Heptadecanoic acid, 15-methyl-, ...	312	C20H40O2	057274-46-1	90
5		Heptadecanoic acid, ethyl ester	298	C19H38O2	014010-23-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112421\
Data File : BM033252.D
Acq On : 24 Nov 2021 18:12
Operator : CG/JU
Sample : M4692-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WW-EFF

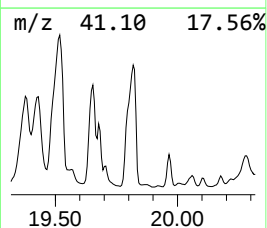
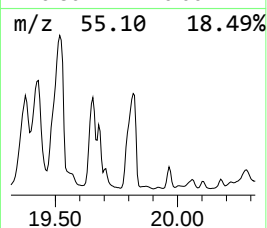
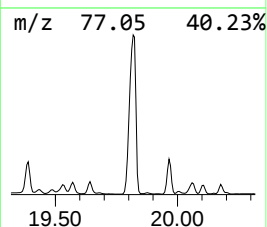
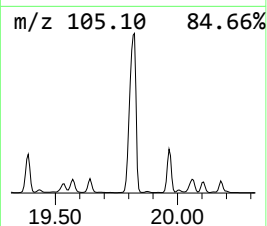
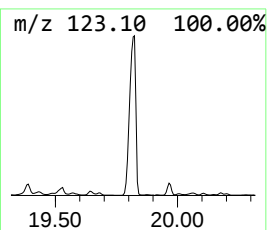
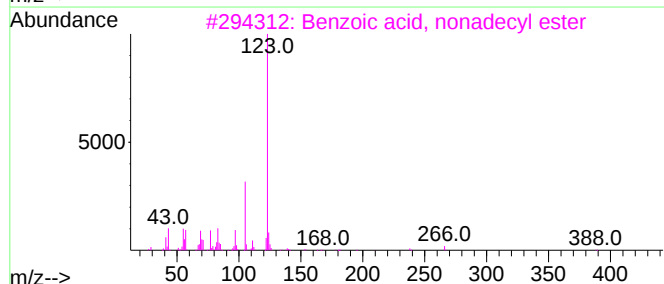
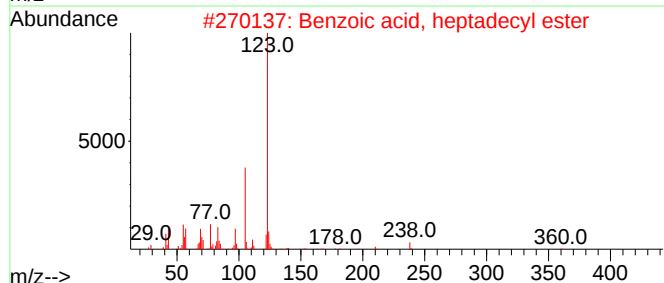
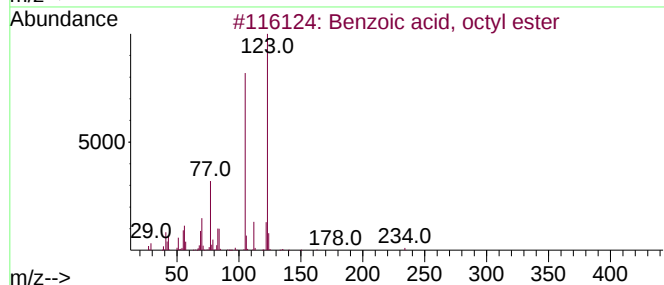
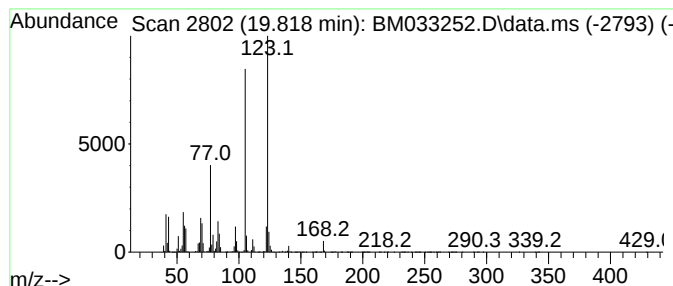
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Benzoic acid, octyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.818	582.89 ng	72375300	Chrysene-d12	21.465

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, octyl ester	234	C15H22O2	000094-50-8	80
2			Benzoic acid, heptadecyl ester	360	C24H40O2	1000340-23-0	72
3			Benzoic acid, nonadecyl ester	388	C26H44O2	1000340-23-2	72
4			2,6-Pyridinedicarboxylic acid	167	C7H5NO4	000499-83-2	72
5			Benzoic acid, octadecyl ester	374	C25H42O2	010578-34-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112421\
Data File : BM033252.D
Acq On : 24 Nov 2021 18:12
Operator : CG/JU
Sample : M4692-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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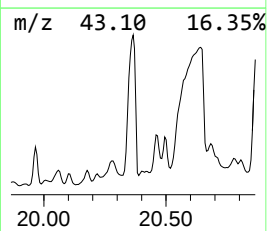
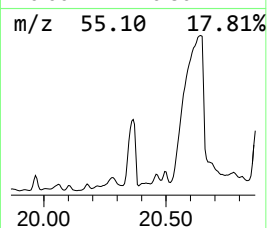
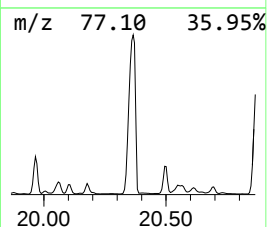
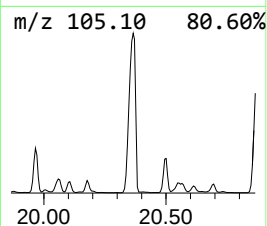
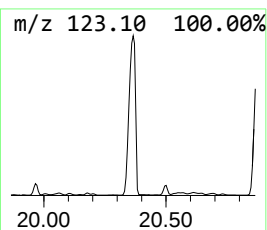
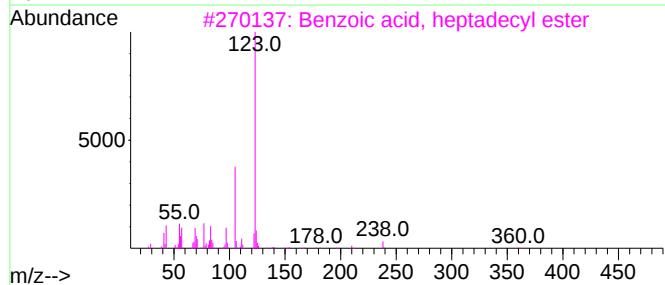
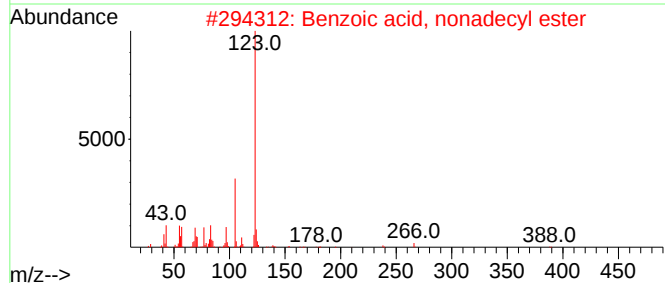
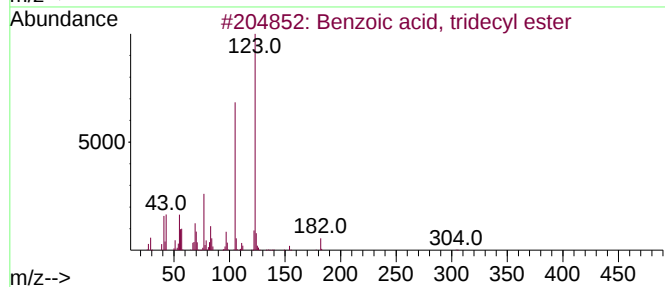
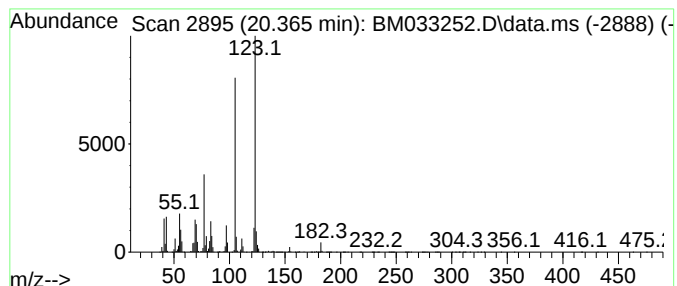
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Benzoic acid, tridecyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.365	499.54 ng	62026100	Chrysene-d12	21.465

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, tridecyl ester	304	C20H32O2	1010340-22-6	91
2			Benzoic acid, nonadecyl ester	388	C26H44O2	1000340-23-2	86
3			Benzoic acid, heptadecyl ester	360	C24H40O2	1000340-23-0	86
4			Benzoic acid, octadecyl ester	374	C25H42O2	010578-34-4	83
5			Eicosyl benzoate	402	C27H46O2	103098-99-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112421\
Data File : BM033252.D
Acq On : 24 Nov 2021 18:12
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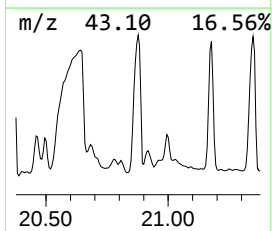
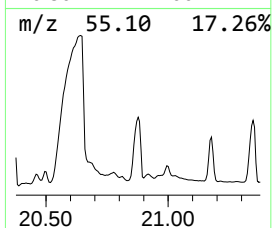
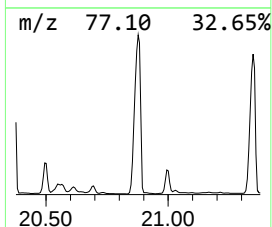
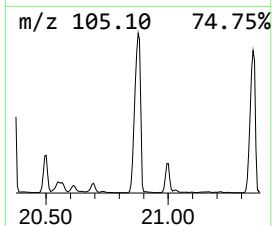
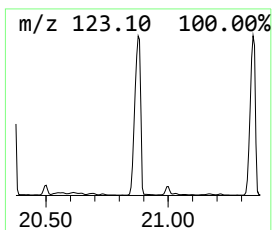
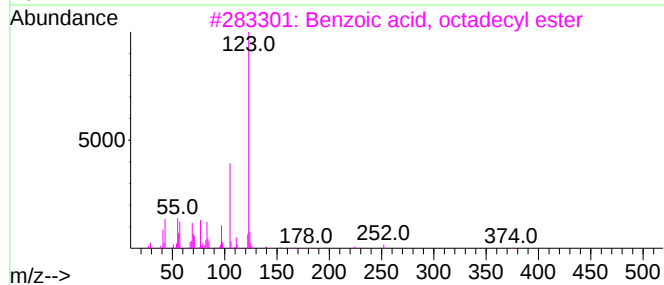
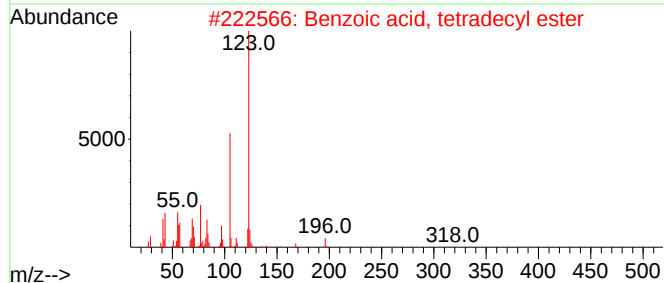
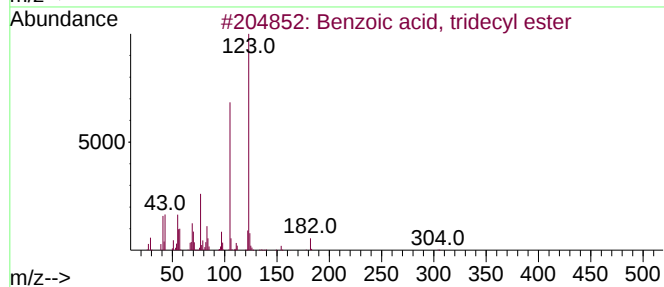
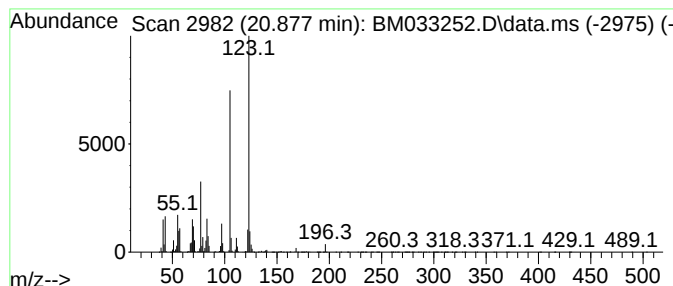
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 Benzoic acid, tetradecyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.877	454.15 ng	56389800	Chrysene-d12	21.465

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, tridecyl ester	304	C20H32O2	1010340-22-6	91
2			Benzoic acid, tetradecyl ester	318	C21H34O2	1000340-22-7	87
3			Benzoic acid, octadecyl ester	374	C25H42O2	010578-34-4	87
4			Benzoic acid, heptadecyl ester	360	C24H40O2	1000340-23-0	86
5			Benzoic acid, undecyl ester	276	C18H28O2	006316-30-9	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112421\
Data File : BM033252.D
Acq On : 24 Nov 2021 18:12
Operator : CG/JU
Sample : M4692-01
Misc :
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ClientSampleId :
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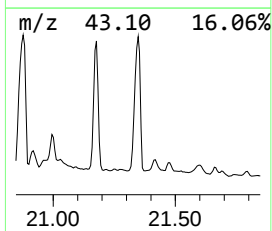
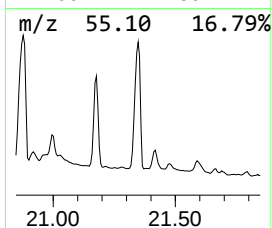
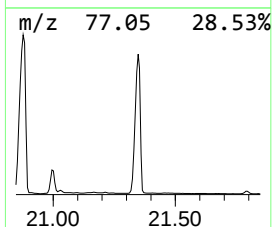
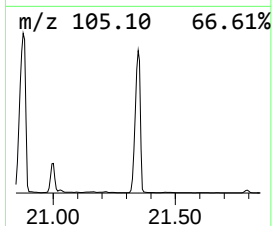
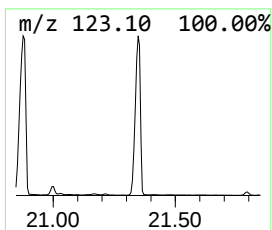
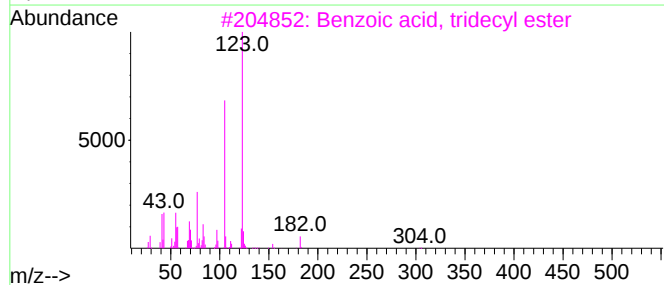
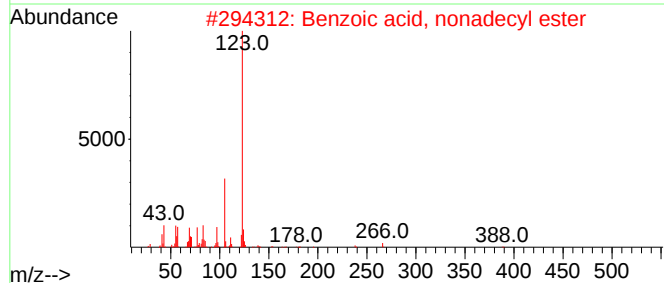
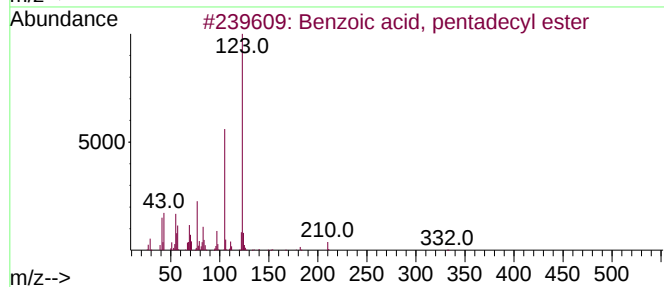
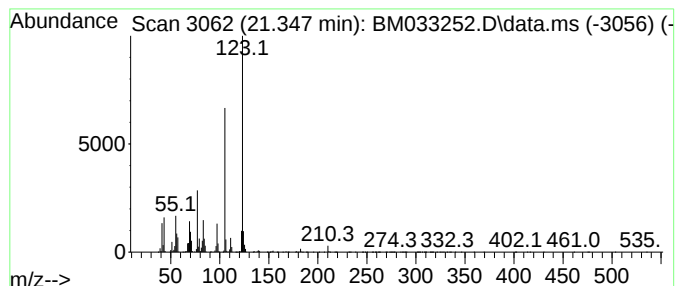
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 Benzoic acid, pentadecyl ester Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.348	356.84 ng	44307600	Chrysene-d12	21.465

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, pentadecyl ester	332	C22H36O2	1000340-22-8	95
2			Benzoic acid, nonadecyl ester	388	C26H44O2	1000340-23-2	91
3			Benzoic acid, tridecyl ester	304	C20H32O2	1010340-22-6	91
4			Benzoic acid, tetradecyl ester	318	C21H34O2	1000340-22-7	91
5			Benzoic acid, octadecyl ester	374	C25H42O2	010578-34-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112421\
Data File : BM033252.D
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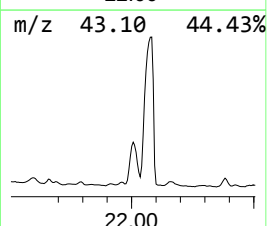
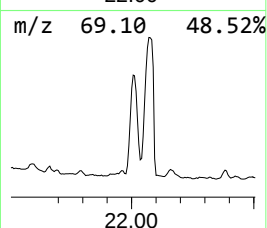
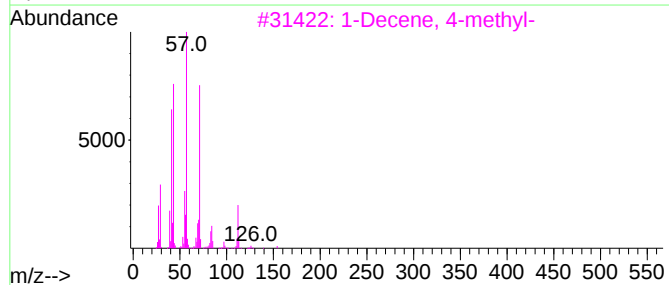
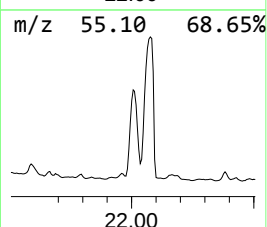
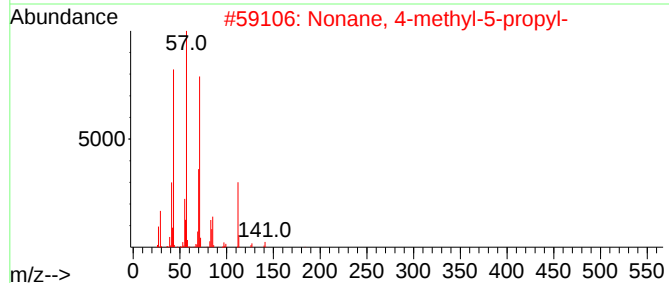
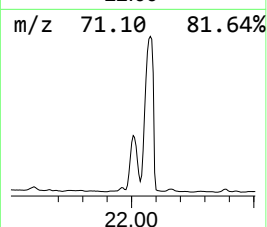
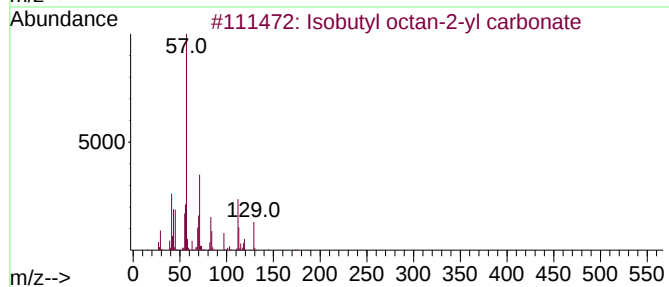
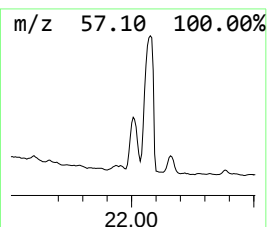
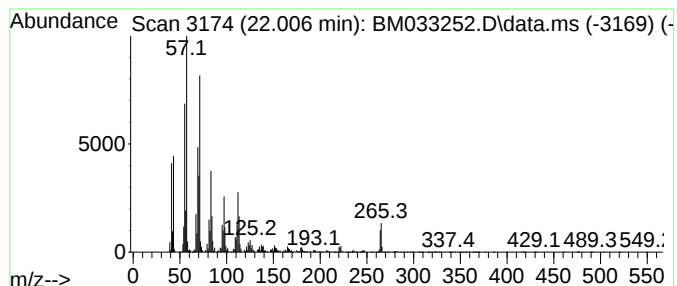
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 Isobutyl octan-2-yl carbonate Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.006	180.58 ng	22421400	Chrysene-d12	21.465

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutyl octan-2-yl carbonate	230	C13H26O3	1000372-74-7	52
2			Nonane, 4-methyl-5-propyl-	184	C13H28	062185-55-1	49
3			1-Decene, 4-methyl-	154	C11H22	013151-29-6	49
4			Heptane, 3-ethyl-5-methyl-	142	C10H22	052896-90-9	43
5			Sulfurous acid, 2-ethylhexyl pen...	264	C13H28O3S	1000309-18-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112421\
Data File : BM033252.D
Acq On : 24 Nov 2021 18:12
Operator : CG/JU
Sample : M4692-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WW-EFF

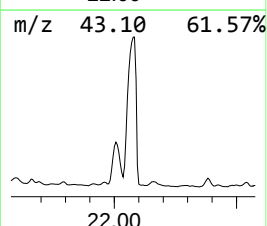
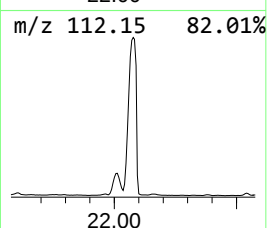
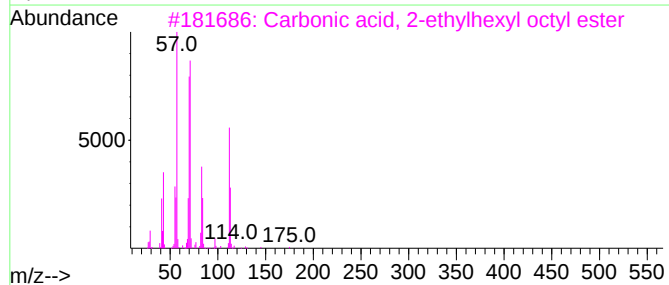
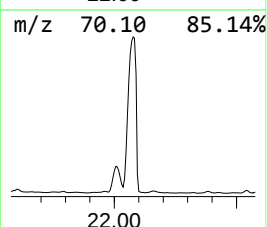
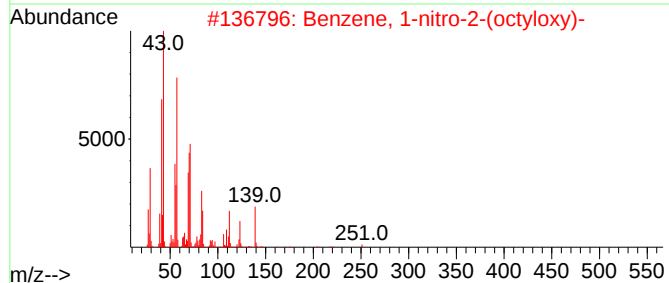
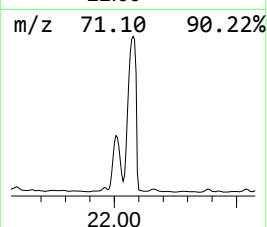
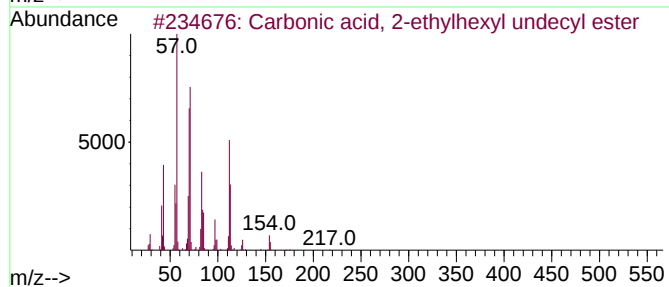
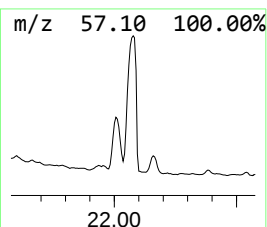
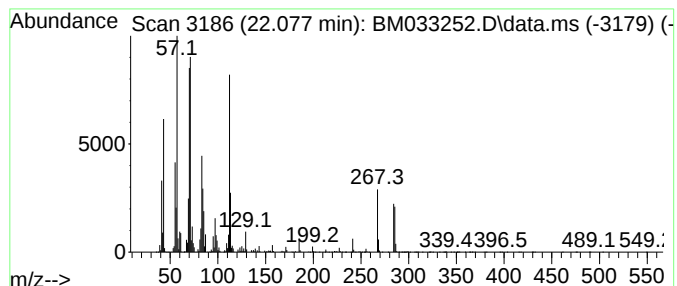
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 Carbonic acid, 2-ethylhexyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.077	570.19 ng	70798100	Chrysene-d12	21.465

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, 2-ethylhexyl unde...	328	C20H40O3	1000383-13-8	70
2			Benzene, 1-nitro-2-(octyloxy)-	251	C14H21NO3	037682-29-4	60
3			Carbonic acid, 2-ethylhexyl octy...	286	C17H34O3	1000383-13-5	58
4			Carbonic acid, 2-ethylhexyl nony...	300	C18H36O3	1000383-13-6	58
5			2-Ethylhexyl stearate	396	C26H52O2	022047-49-0	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112421\
Data File : BM033252.D
Acq On : 24 Nov 2021 18:12
Operator : CG/JU
Sample : M4692-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WW-EFF

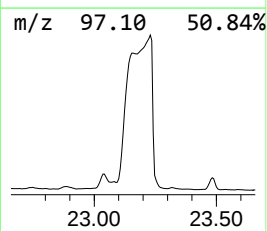
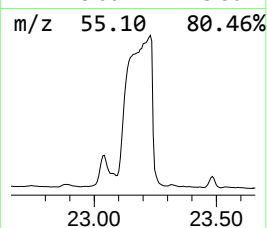
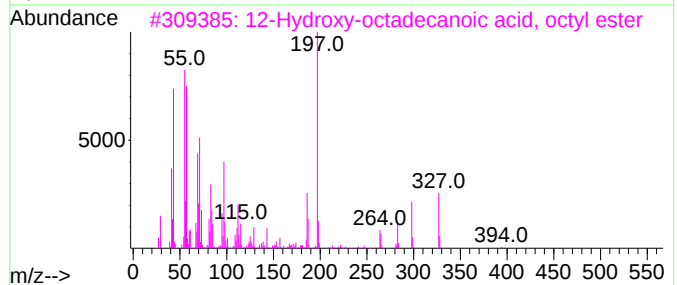
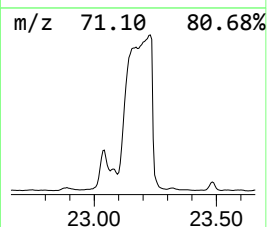
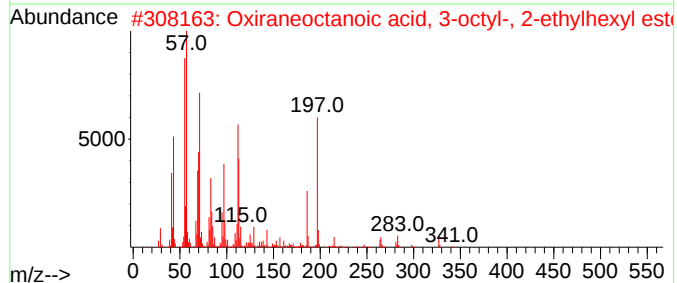
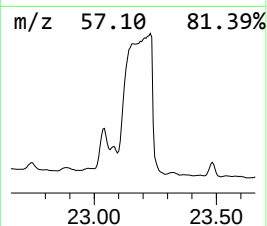
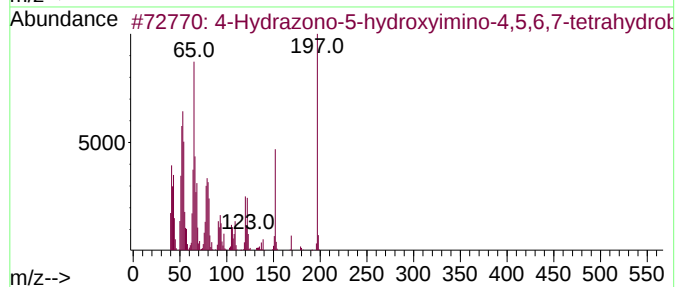
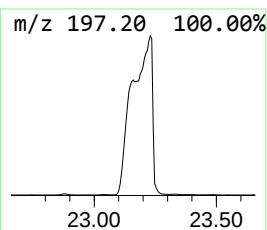
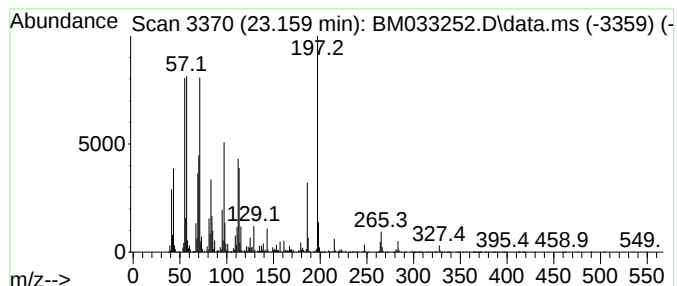
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 4-Hydrazono-5-hydroxyimino-... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.159	336.51 ng	84543500	Perylene-d12	23.806

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Hydrazono-5-hydroxyimino-4,5,6...	197	C6H7N5O3	303194-86-7	90
2			Oxiraneoctanoic acid, 3-octyl-, ...	410	C26H50O3	000141-38-8	59
3			12-Hydroxy-octadecanoic acid, oc...	412	C26H52O3	074819-90-2	47
4			Carbonic acid, 2-ethylhexyl hexa...	398	C25H50O3	1000383-14-3	35
5			Carbonic acid, 2-ethylhexyl hept...	412	C26H52O3	1000383-14-4	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112421\
Data File : BM033252.D
Acq On : 24 Nov 2021 18:12
Operator : CG/JU
Sample : M4692-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WW-EFF

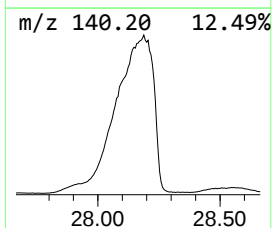
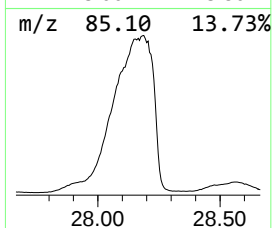
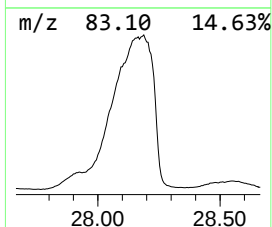
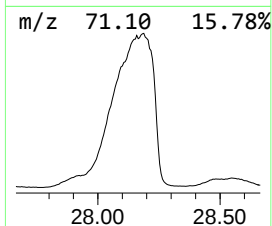
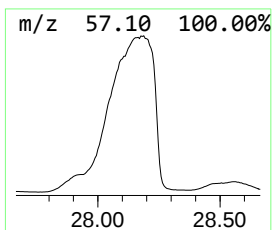
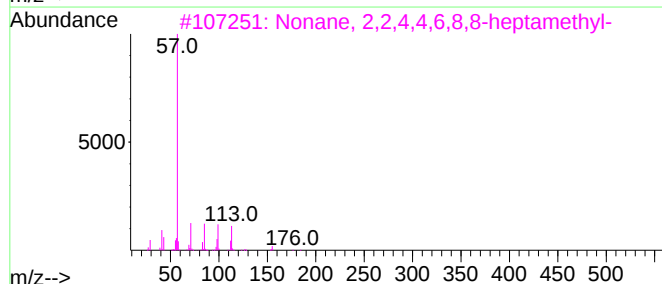
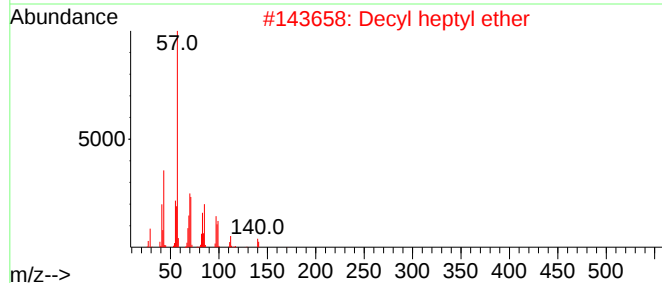
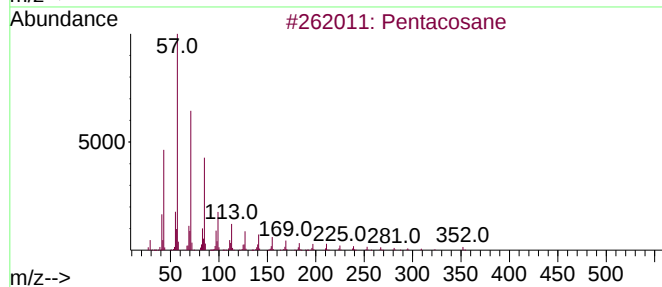
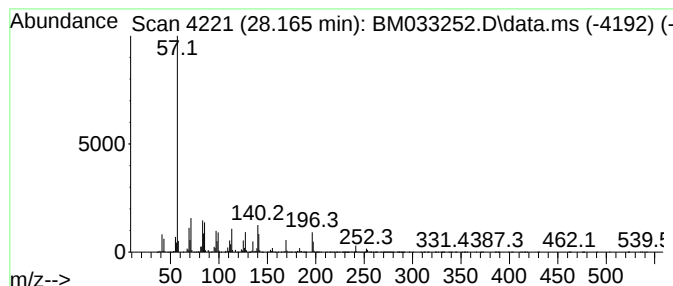
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 Pentacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.165	481.33 ng	120926000	Perylene-d12	23.806

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentacosane	352	C25H52	000629-99-2	38
2		Decyl heptyl ether	256	C17H36O	1000406-39-1	38
3		Nonane, 2,2,4,4,6,8,8-heptamethyl-	226	C16H34	004390-04-9	38
4		2,2,4,4,5,5,7,7-Octamethyloctane	226	C16H34	005171-85-7	35
5		Octanoic acid, 2-propenyl ester	184	C11H20O2	004230-97-1	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM112421\
 Data File : BM033252.D
 Acq On : 24 Nov 2021 18:12
 Operator : CG/JU
 Sample : M4692-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 WW-EFF

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Decene	14.224	349.5	ng	58255800	3	14.560	3333790	20.0
Trichloroacetic...	15.213	1059.3	ng	176570000	3	14.560	3333790	20.0
1-Dodecene	16.101	262.8	ng	24400400	4	17.307	1856730	20.0
1-Octanol, 5,7,...	16.489	695.0	ng	64525500	4	17.307	1856730	20.0
Carbonic acid, ...	16.613	744.7	ng	69136700	4	17.307	1856730	20.0
Tetradecanoic acid	16.754	333.8	ng	30988000	4	17.307	1856730	20.0
1-Hexacosene	16.789	166.1	ng	15418600	4	17.307	1856730	20.0
n-Hexadecanoic ...	18.224	438.6	ng	40717800	4	17.307	1856730	20.0
trans-13-Octade...	19.383	446.0	ng	41407900	4	17.307	1856730	20.0
6-Octadecenoic ...	19.430	195.0	ng	24216500	5	21.465	2483330	20.0
Octadecanoic acid	19.518	591.4	ng	73428100	5	21.465	2483330	20.0
Octadecanoic ac...	19.654	326.3	ng	40511100	5	21.465	2483330	20.0
Benzoic acid, o...	19.818	582.9	ng	72375300	5	21.465	2483330	20.0
Benzoic acid, t...	20.365	499.5	ng	62026100	5	21.465	2483330	20.0
Benzoic acid, t...	20.877	454.1	ng	56389800	5	21.465	2483330	20.0
Benzoic acid, p...	21.348	356.8	ng	44307600	5	21.465	2483330	20.0
Isobutyl octan-...	22.006	180.6	ng	22421400	5	21.465	2483330	20.0
Carbonic acid, ...	22.077	570.2	ng	70798100	5	21.465	2483330	20.0
4-Hydrazono-5-h...	23.159	336.5	ng	84543500	6	23.806	5024670	20.0
Pentacosane	28.165	481.3	ng	120926000	6	23.806	5024670	20.0