

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031324\
 Data File : BM044607.D
 Acq On : 13 Mar 2024 21:00
 Operator : MA/JU
 Sample : P1723-02
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 EFF-WW

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-BM031324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM044607.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.599	421	427	454	rVV	986266	4735714	2.06%	0.395%
2	6.616	589	600	619	rBV2	960252	2440797	1.06%	0.203%
3	7.798	789	801	818	rBV2	20041743	158257777	68.94%	13.192%
4	8.581	906	934	937	rVB	2138573	11172909	4.87%	0.931%
5	8.928	984	993	1010	rVB	1750333	4458099	1.94%	0.372%
6	9.316	1011	1059	1062	rBV	4637556	32855414	14.31%	2.739%
7	10.210	1154	1211	1212	rBV4	6780539	67349723	29.34%	5.614%
8	10.463	1247	1254	1258	rBV	1316816	2954796	1.29%	0.246%
9	12.828	1618	1656	1660	rBV	9537731	62912056	27.40%	5.244%
10	12.975	1674	1681	1685	rBV	5359164	8763987	3.82%	0.731%
11	13.033	1685	1691	1704	rVB	3136533	6137804	2.67%	0.512%
12	14.010	1851	1857	1865	rBV3	1301248	2443511	1.06%	0.204%
13	14.351	1906	1915	1924	rVV	1868887	2898508	1.26%	0.242%
14	15.051	1984	2034	2039	rBV6	19628844	229565967	100.00%	19.136%
15	15.851	2163	2170	2177	rBV3	2677366	4886542	2.13%	0.407%
16	15.916	2177	2181	2194	rVB	1680370	2657283	1.16%	0.222%
17	16.286	2237	2244	2248	rBV	12798860	22001243	9.58%	1.834%
18	16.333	2248	2252	2257	rVV	19940023	37780852	16.46%	3.149%
19	16.386	2257	2261	2273	rVV	15734061	26230808	11.43%	2.187%
20	16.586	2277	2295	2311	rVV	14448884	43867074	19.11%	3.657%
21	16.886	2341	2346	2361	rVB2	1641629	3488565	1.52%	0.291%
22	17.104	2378	2383	2390	rVB2	1946383	3063702	1.33%	0.255%
23	18.027	2534	2540	2561	rBV	6748139	14803433	6.45%	1.234%
24	18.451	2607	2612	2614	rBV2	1624454	2365796	1.03%	0.197%
25	18.504	2614	2621	2625	rVV	10318636	19988317	8.71%	1.666%
26	18.562	2625	2631	2651	rVV	3141392	12819274	5.58%	1.069%
27	18.951	2692	2697	2705	rVB	5627606	8685802	3.78%	0.724%
28	19.192	2734	2738	2741	rBV	3106888	4677366	2.04%	0.390%
29	19.362	2763	2767	2772	rVB2	3299722	4132115	1.80%	0.344%
30	19.492	2785	2789	2791	rBV2	4260591	5385817	2.35%	0.449%
31	19.521	2791	2794	2797	rVB	3895818	4640892	2.02%	0.387%
32	19.651	2811	2816	2826	rVB2	13339035	19555544	8.52%	1.630%
33	19.751	2828	2833	2835	rBV	8701447	14437824	6.29%	1.204%
34	19.815	2840	2844	2849	rVB2	1983792	3042675	1.33%	0.254%
35	20.068	2884	2887	2893	rVB	4287318	5086515	2.22%	0.424%
36	20.209	2906	2911	2915	rBV	10876553	14414245	6.28%	1.202%

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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

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37	20.721	2994	2998	3002	rVB	10156306	12287899	5.35%	1.024%
38	20.892	3013	3027	3031	rVB	14411832	51733668	22.54%	4.312%
39	21.045	3048	3053	3057	rBV	8856497	10999674	4.79%	0.917%
40	21.203	3076	3080	3085	rBV	10729120	12559421	5.47%	1.047%
41	21.839	3177	3188	3191	rBV3	15322465	33676378	14.67%	2.807%
42	21.868	3191	3193	3198	rVV	2273832	3177368	1.38%	0.265%
43	21.927	3198	3203	3210	rVB	14788577	21874847	9.53%	1.823%
44	22.239	3252	3256	3269	rVB	2721183	4619980	2.01%	0.385%
45	22.868	3359	3363	3367	rVB	2111407	3000011	1.31%	0.250%
46	22.974	3368	3381	3383	rBV4	17227099	47153605	20.54%	3.931%
47	23.080	3394	3399	3415	rVB	4280526	7165791	3.12%	0.597%
48	23.297	3429	3436	3443	rBV	8121689	14413333	6.28%	1.201%
49	23.550	3473	3479	3493	rVB2	1821001	3880267	1.69%	0.323%
50	24.291	3597	3605	3619	rVB	5743452	13242323	5.77%	1.104%
51	24.797	3682	3691	3704	rVB	7687361	18275504	7.96%	1.523%
52	25.891	3869	3877	3886	rBV2	2068431	5724024	2.49%	0.477%
53	26.333	3943	3952	3964	rVB	1685745	4963744	2.16%	0.414%
54	26.527	3977	3985	3991	rBV2	2003584	6103971	2.66%	0.509%
55	26.674	4003	4010	4027	rVB	4013259	12395995	5.40%	1.033%
56	27.703	4165	4185	4186	rBV	6438300	26775831	11.66%	2.232%
57	28.979	4389	4402	4419	rVB2	2541352	10656497	4.64%	0.888%

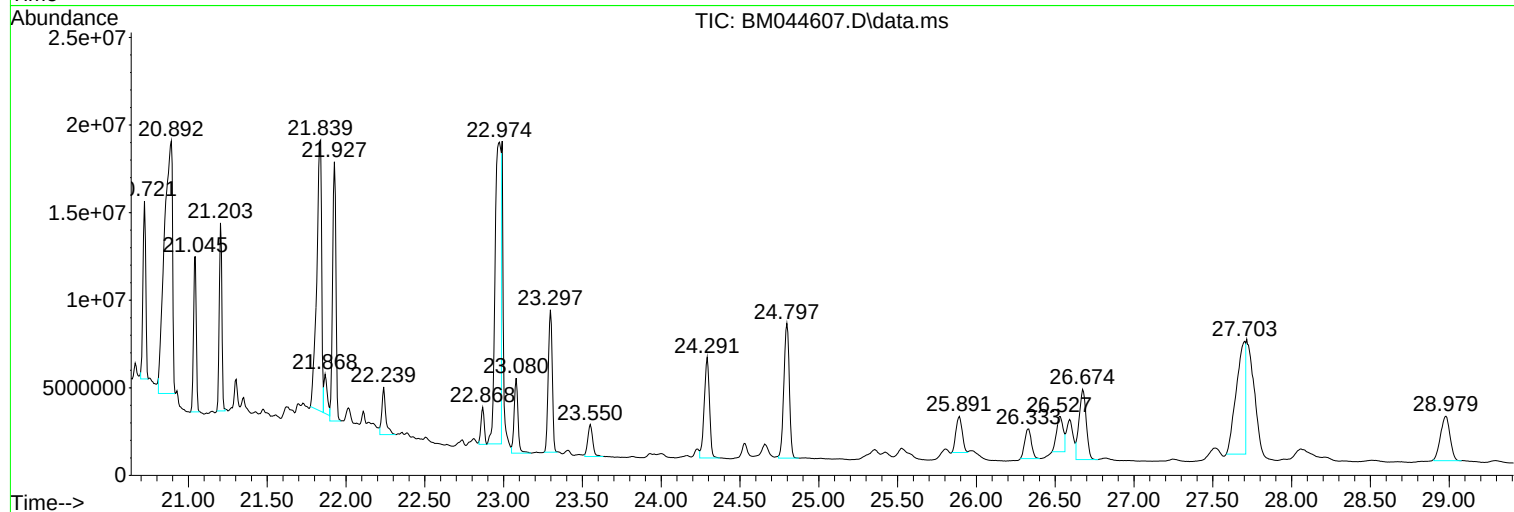
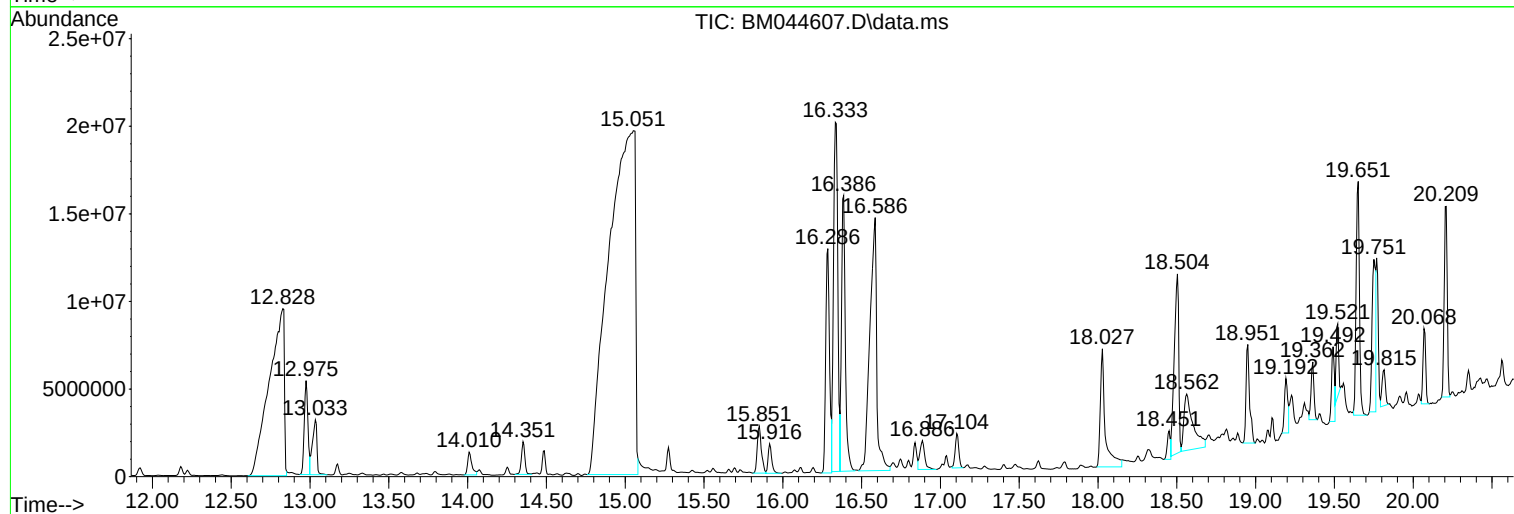
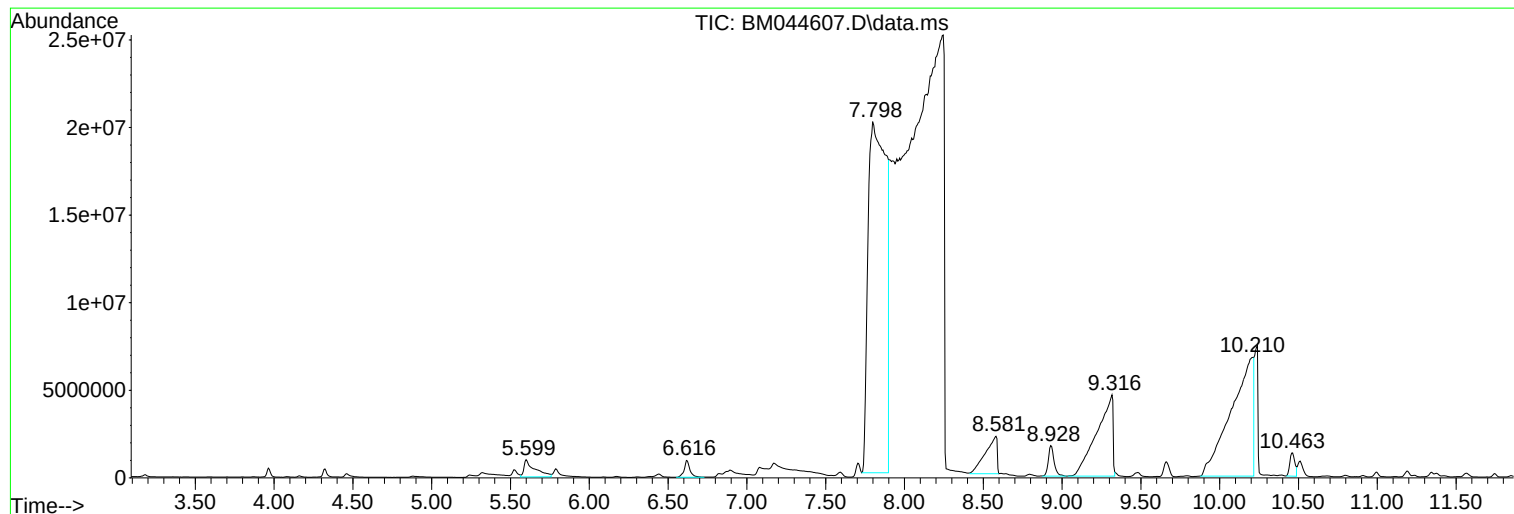
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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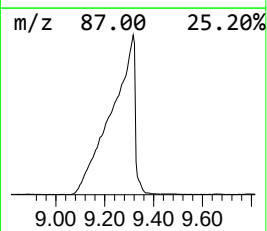
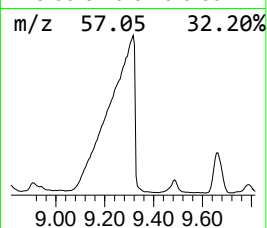
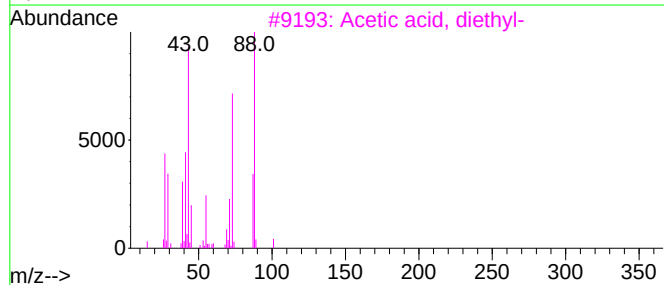
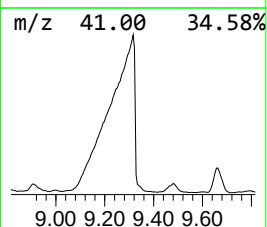
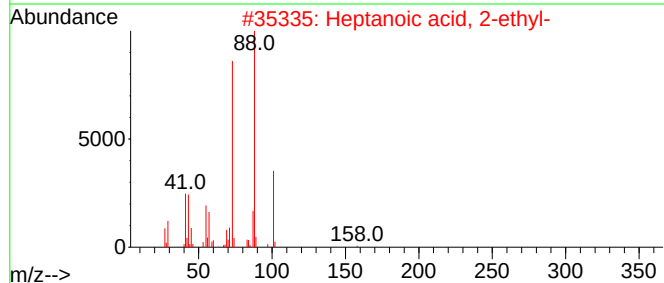
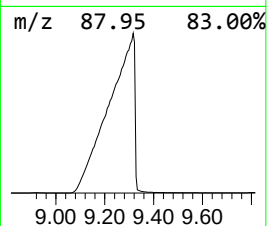
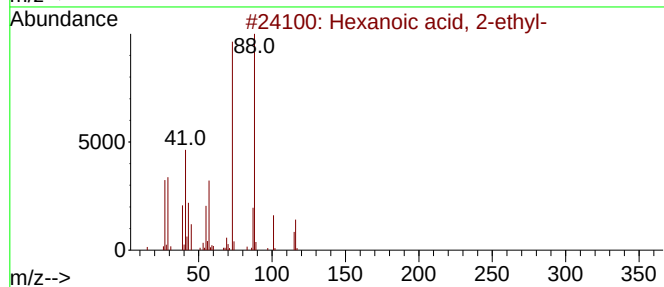
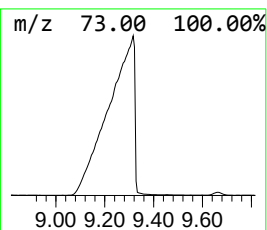
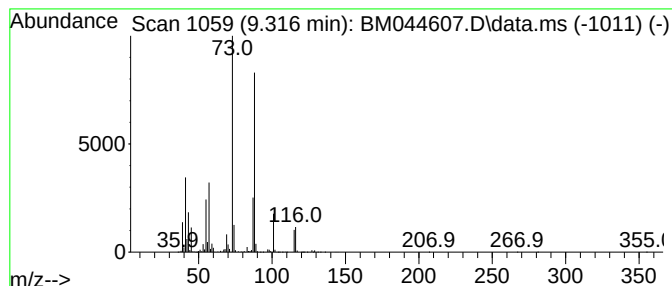
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hexanoic acid, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.316	222.39 ng	32855400	Naphthalene-d8	10.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
2			Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	53
3			Acetic acid, diethyl-	116	C6H12O2	000088-09-5	53
4			2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	50
5			Octanoic acid, 2-methyl-, methyl...	172	C10H20O2	002177-86-8	43



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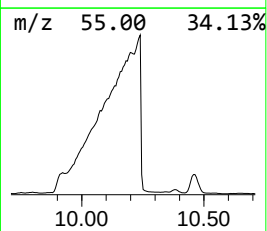
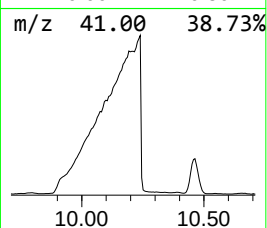
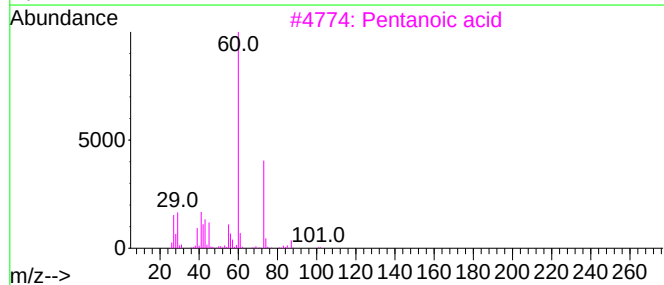
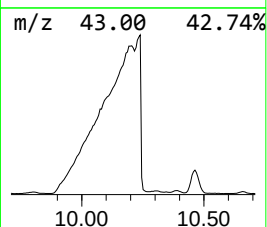
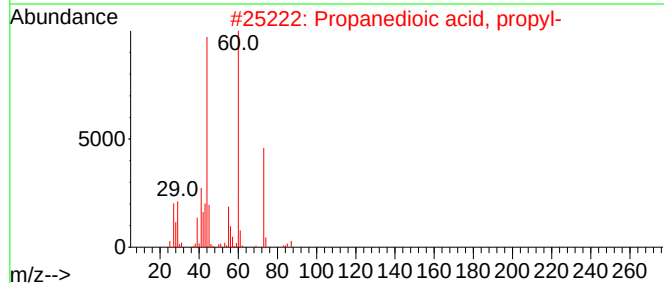
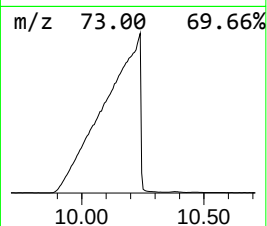
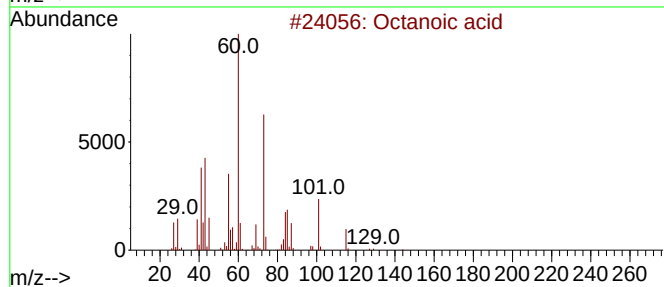
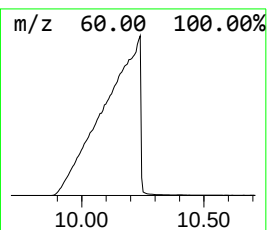
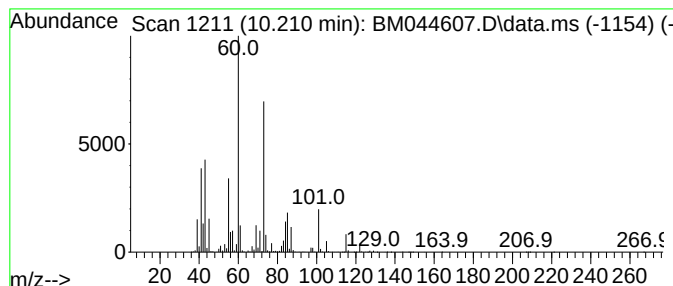
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Octanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.210	455.87 ng	67349700	Naphthalene-d8	10.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octanoic acid	144	C8H16O2	000124-07-2	97
2			Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	50
3			Pentanoic acid	102	C5H10O2	000109-52-4	50
4			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	50
5			Hexanoic acid	116	C6H12O2	000142-62-1	49



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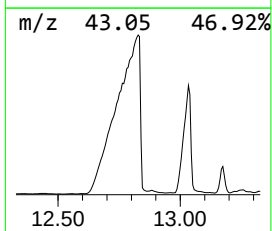
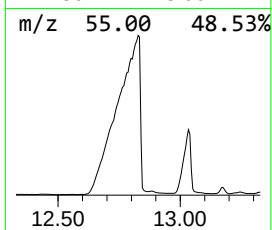
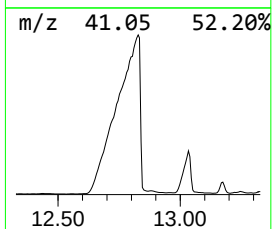
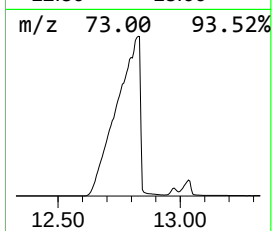
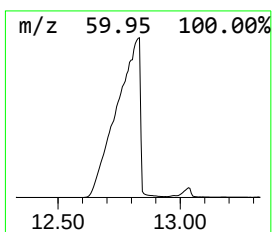
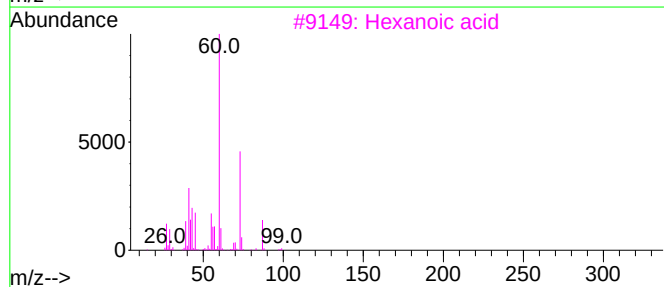
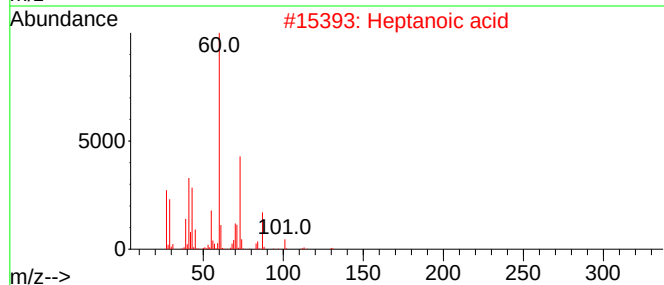
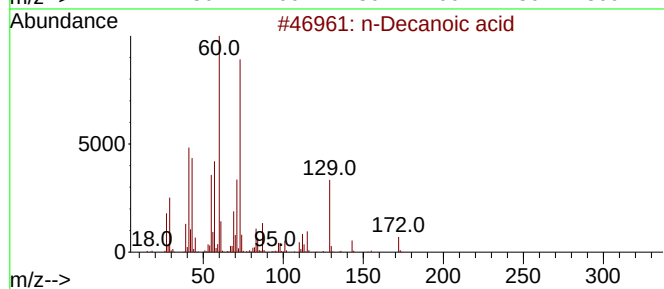
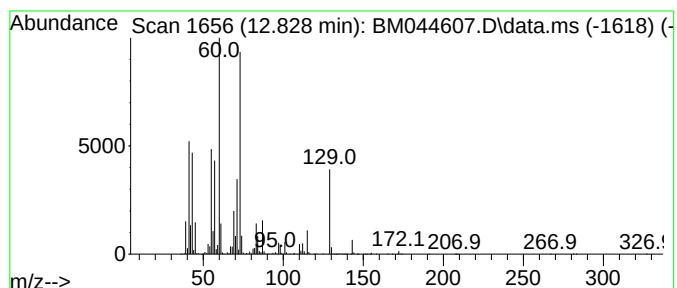
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Decanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.828	434.10 ng	62912100	Acenaphthene-d10	14.351	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	91
2	Heptanoic acid	130	C7H14O2	000111-14-8	47
3	Hexanoic acid	116	C6H12O2	000142-62-1	47
4	Octanoic acid	144	C8H16O2	000124-07-2	47
5	Pentanoic acid	102	C5H10O2	000109-52-4	43



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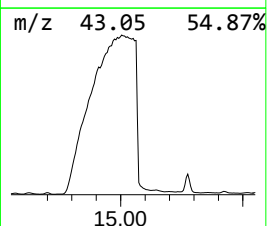
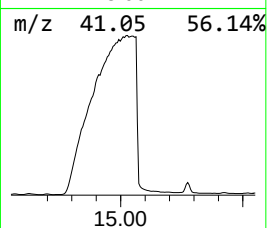
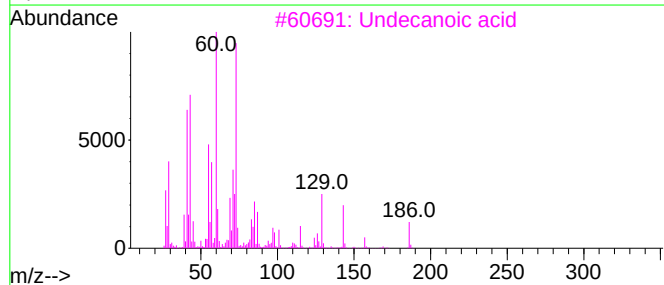
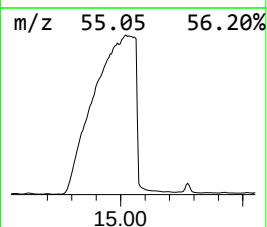
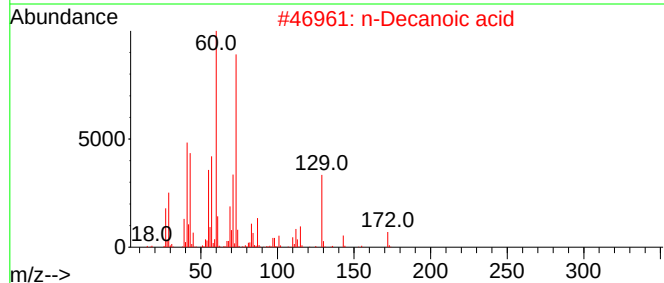
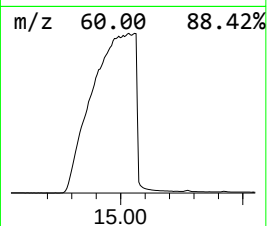
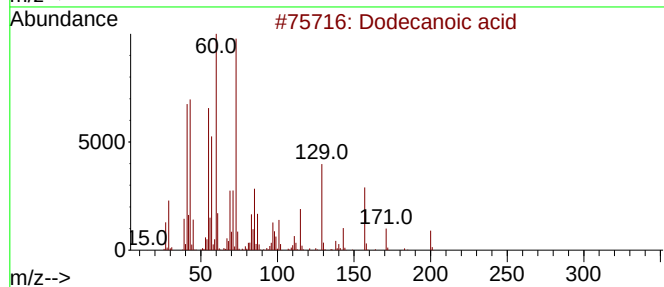
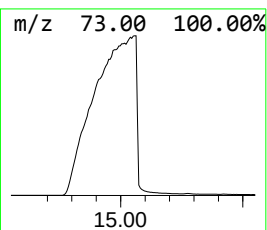
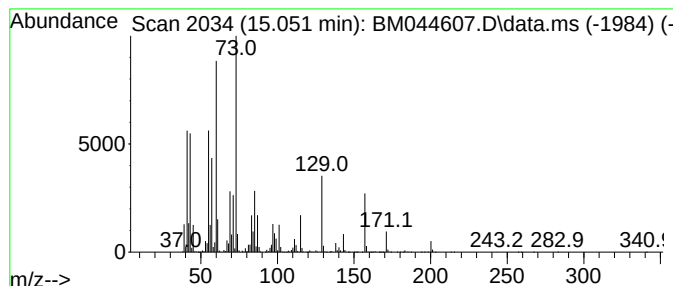
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Dodecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.051	1584.03 ng	229566000	Acenaphthene-d10	14.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	98
2			n-Decanoic acid	172	C10H20O2	000334-48-5	62
3			Undecanoic acid	186	C11H22O2	000112-37-8	59
4			Octanoic acid	144	C8H16O2	000124-07-2	49
5			Nonanoic acid	158	C9H18O2	000112-05-0	46



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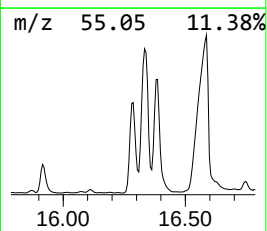
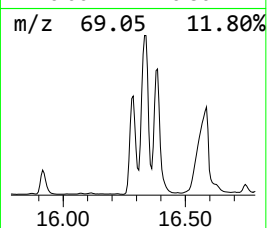
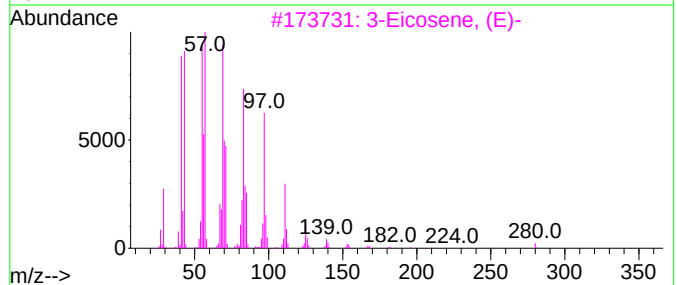
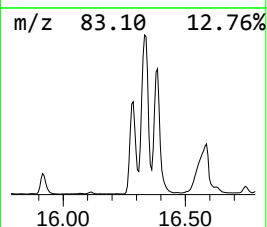
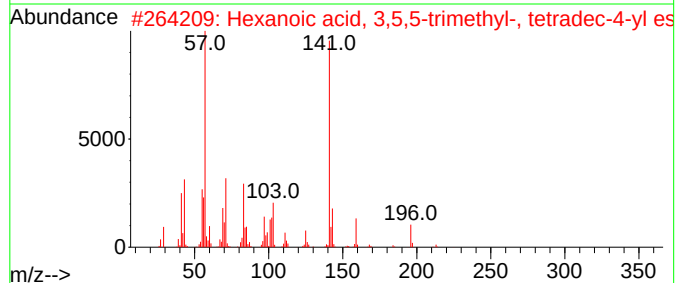
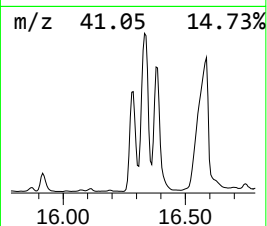
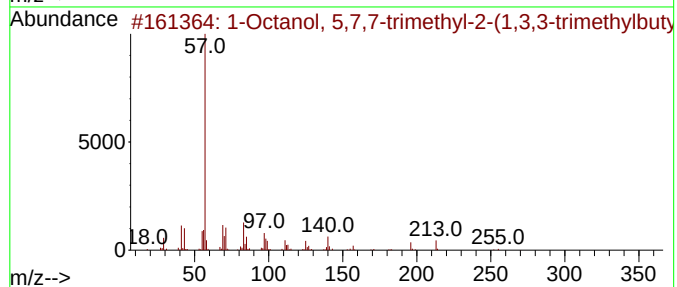
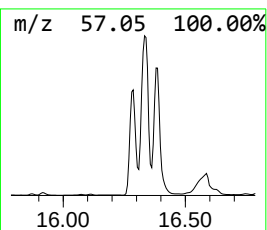
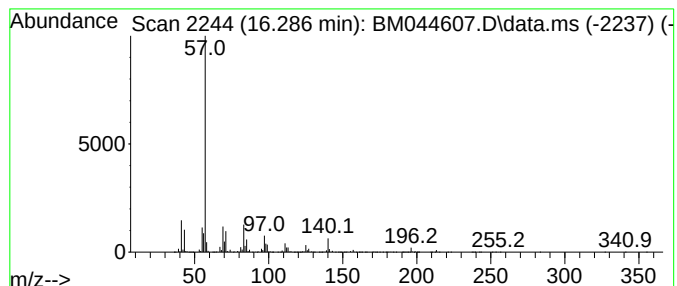
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Octanol, 5,7,7-trimethyl-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.286	143.63 ng	22001200	Phenanthrene-d10	17.104

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		Hexanoic acid, 3,5,5-trimethyl-,...	354	C23H46O2	1000406-26-8	50
3		3-Eicosene, (E)-	280	C20H40	074685-33-9	50
4		1-Dodecanol, 3,7,11-trimethyl-	228	C15H32O	006750-34-1	50
5		Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031324\
Data File : BM044607.D
Acq On : 13 Mar 2024 21:00
Operator : MA/JU
Sample : P1723-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EFF-WW

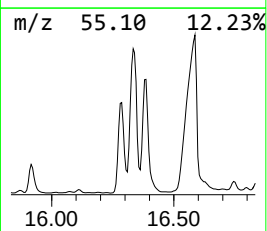
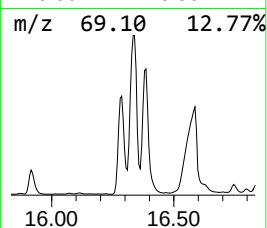
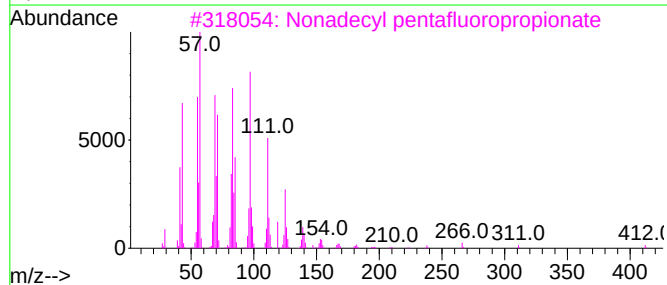
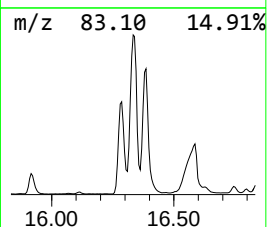
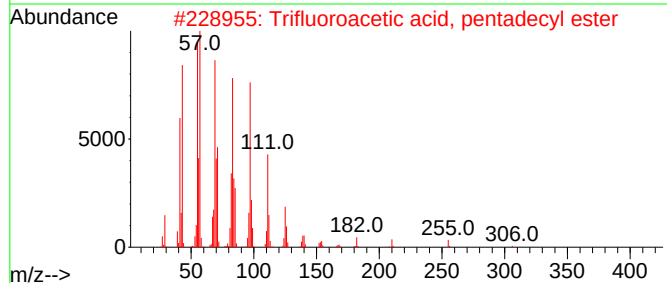
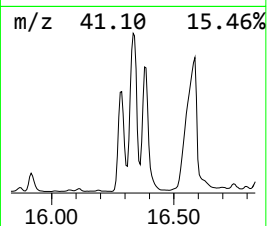
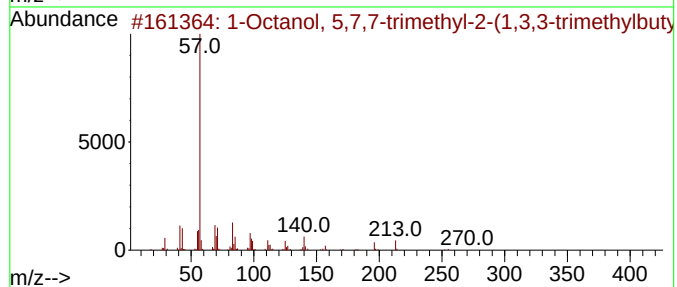
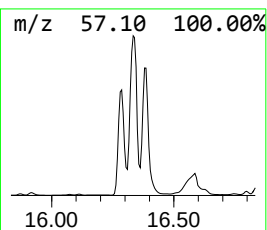
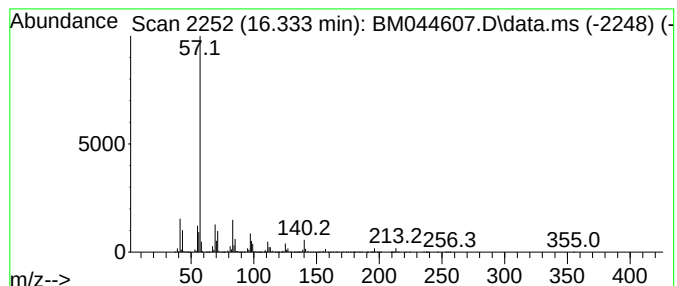
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Trifluoroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.333	246.63 ng	37780900	Phenanthrene-d10	17.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octanol, 5,7,7-trimethyl-2-(1,...	270	C18H38O	036400-98-3	90
2			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	50
3			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	47
4			1-Dodecanol, 3,7,11-trimethyl-	228	C15H32O	006750-34-1	47
5			Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031324\
Data File : BM044607.D
Acq On : 13 Mar 2024 21:00
Operator : MA/JU
Sample : P1723-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
EFF-WW

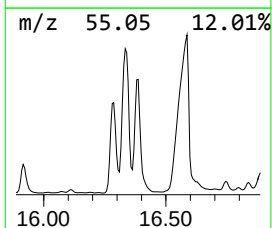
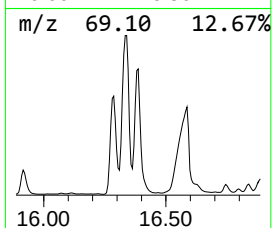
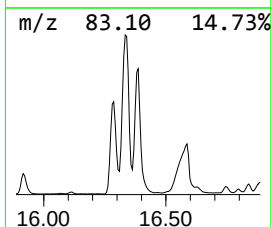
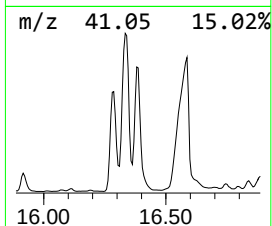
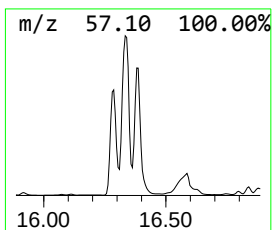
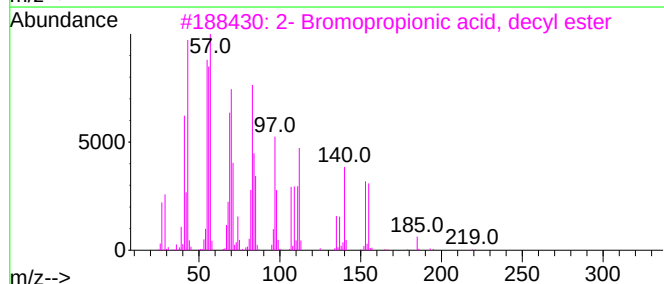
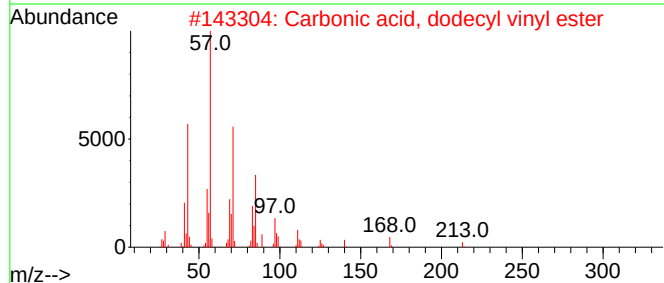
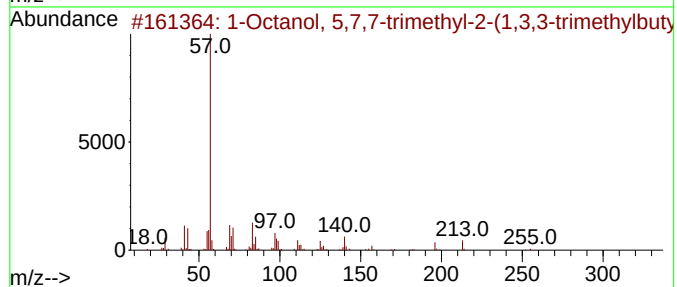
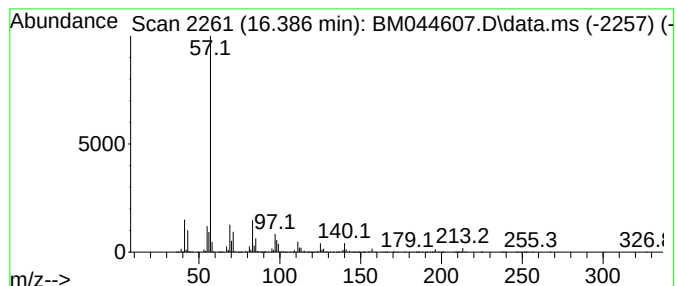
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Carbonic acid, dodecyl vinyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.386	171.24 ng	26230800	Phenanthrene-d10	17.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol, 5,7,7-trimethyl-2-(1,...	270	C18H38O	036400-98-3	72		
2	Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	59		
3	2- Bromopropionic acid, decyl ester	292	C13H25BrO2	026072-74-2	50		
4	Carbonic acid, but-2-yn-1-yl pen...	324	C20H36O3	1010383-21-0	50		
5	Carbonic acid, but-2-yn-1-yl eic...	394	C25H46O3	1000383-21-4	50		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031324\
Data File : BM044607.D
Acq On : 13 Mar 2024 21:00
Operator : MA/JU
Sample : P1723-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
EFF-WW

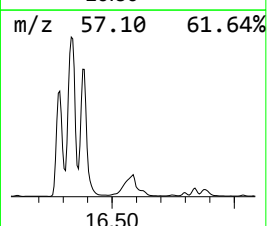
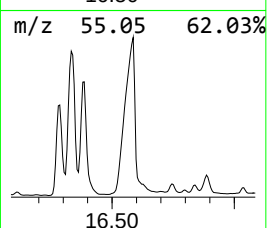
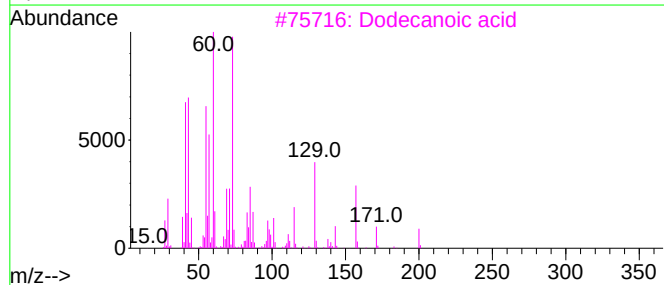
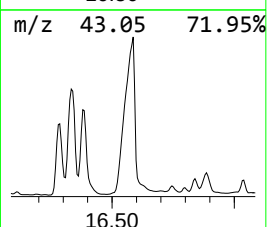
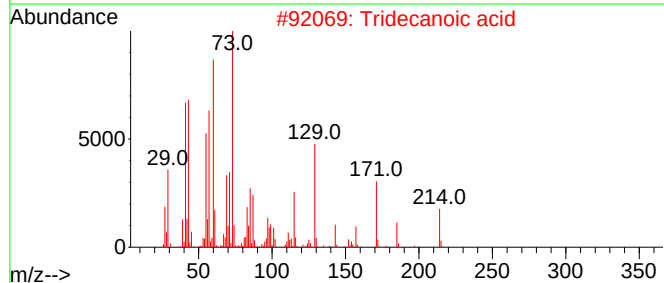
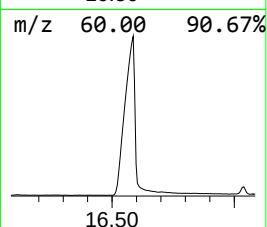
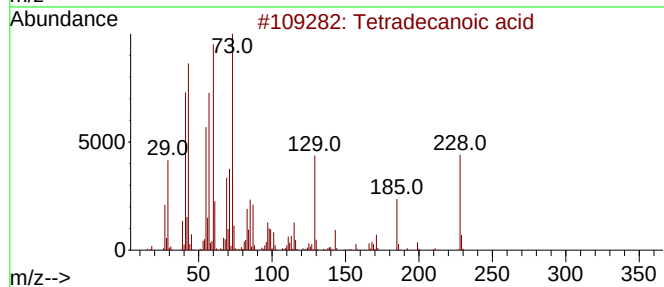
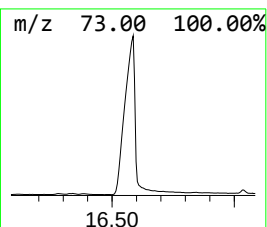
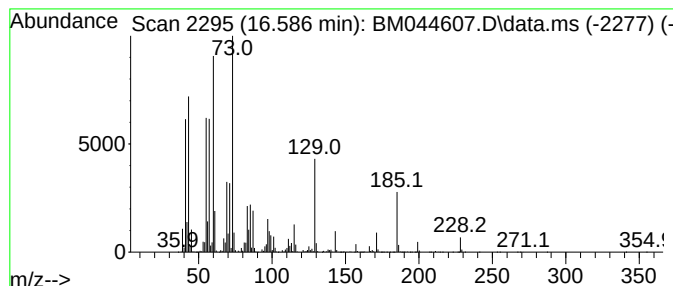
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetradecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.586	286.37 ng	43867100	Phenanthrene-d10	17.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	95
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Dodecanoic acid	200	C12H24O2	000143-07-7	80
4			n-Decanoic acid	172	C10H20O2	000334-48-5	76
5			Undecanoic acid	186	C11H22O2	000112-37-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031324\
Data File : BM044607.D
Acq On : 13 Mar 2024 21:00
Operator : MA/JU
Sample : P1723-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

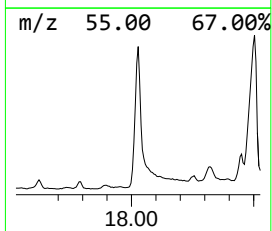
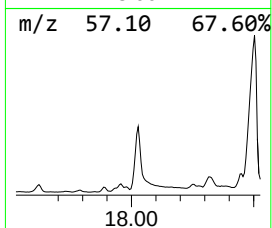
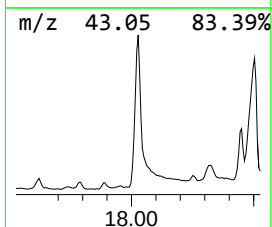
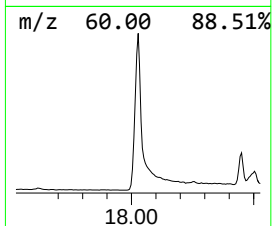
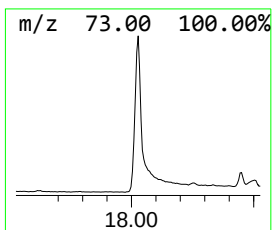
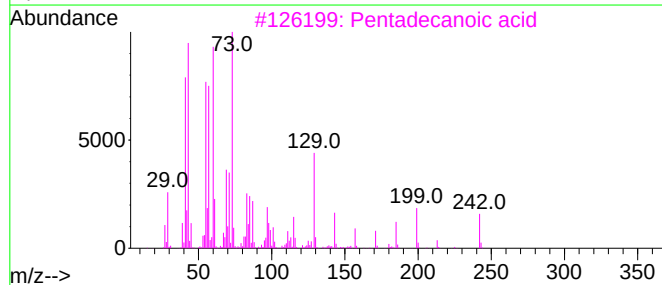
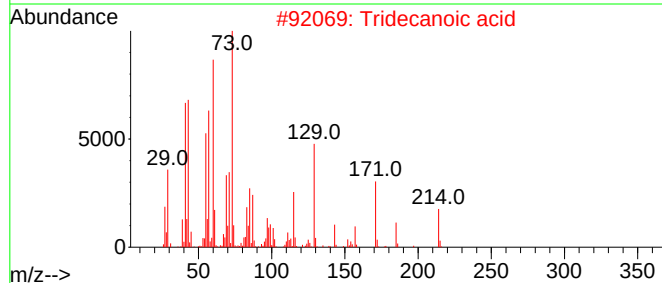
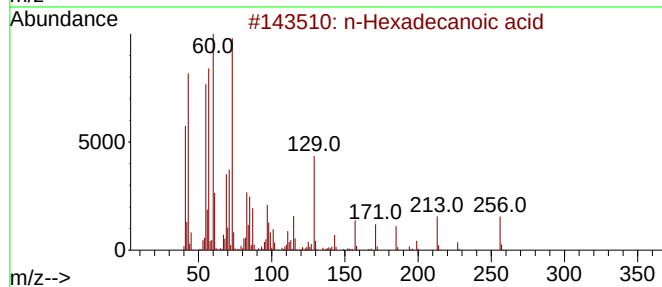
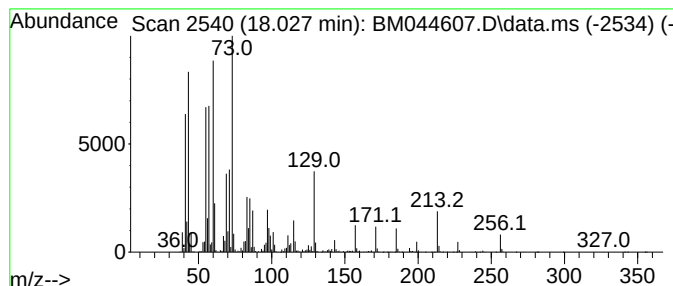
Instrument :
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ClientSampleId :
EFF-WW

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.027	96.64 ng	14803400	Phenanthrene-d10	17.104	
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	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031324\
Data File : BM044607.D
Acq On : 13 Mar 2024 21:00
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Sample : P1723-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

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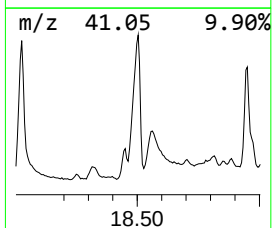
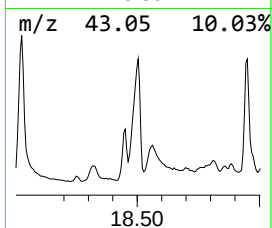
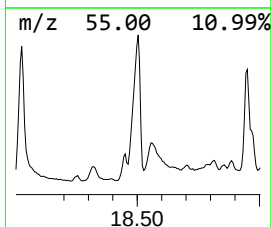
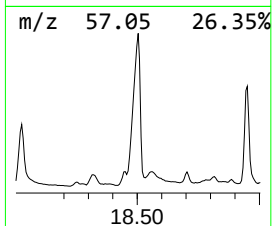
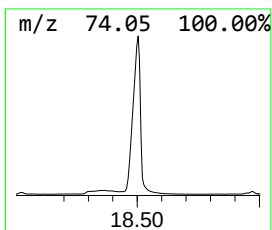
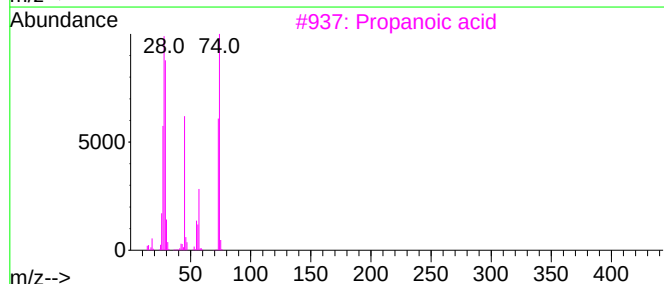
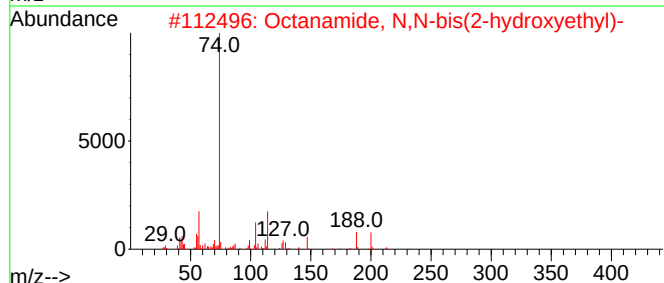
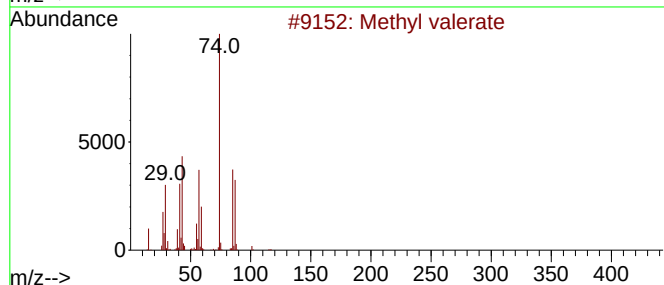
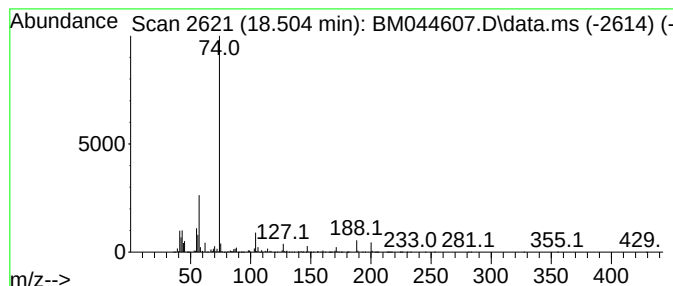
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Methyl valerate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.504	130.49 ng	19988300	Phenanthrene-d10	17.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl valerate	116	C6H12O2	000624-24-8	50
2			Octanamide, N,N-bis(2-hydroxyeth...	231	C12H25NO3	003077-30-3	43
3			Propanoic acid	74	C3H6O2	000079-09-4	40
4			Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	33
5			2-Amino-4-methyl-4-pentenoic acid	129	C6H11NO2	1010133-00-5	33



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031324\
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Misc :
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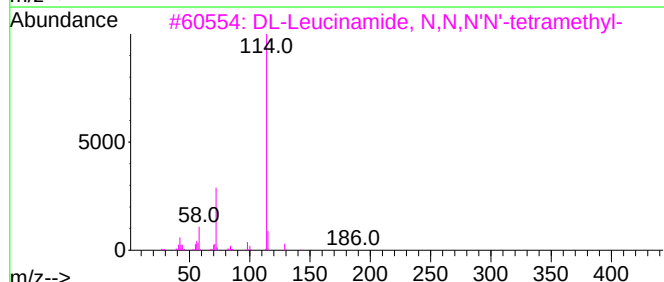
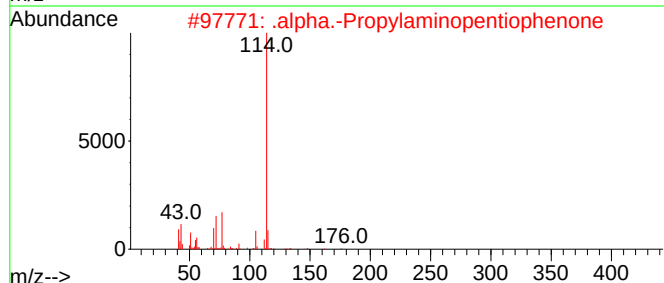
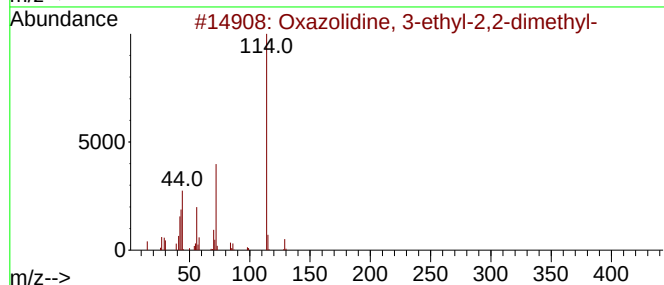
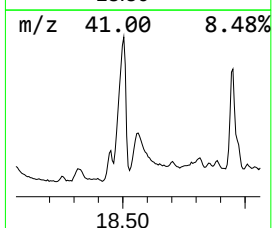
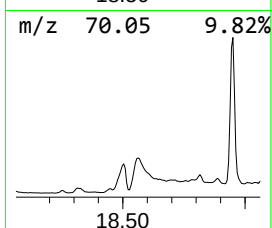
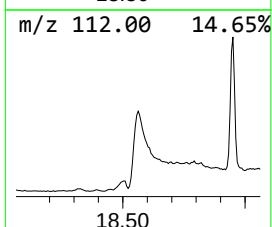
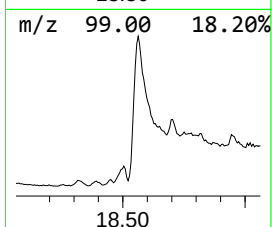
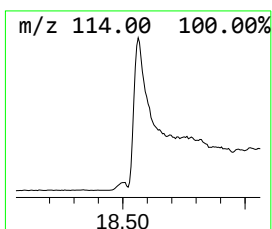
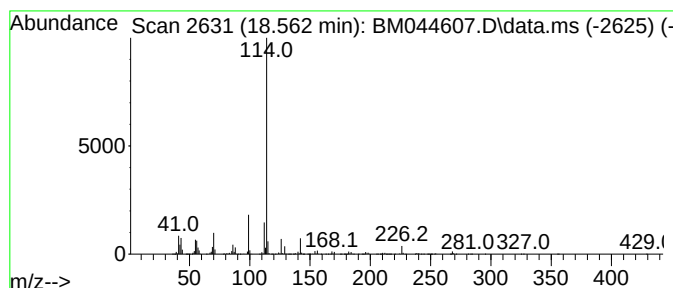
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Oxazolidine, 3-ethyl-2,2-di... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD			R.T.
18.562	83.68 ng	12819300	Phenanthrene-d10			17.104
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Oxazolidine, 3-ethyl-2,2-dimethyl-		129	C7H15NO	057817-78-4	50
2	.alpha.-Propylaminopentiophenone		219	C14H21NO	747345-91-1	40
3	DL-Leucinamide, N,N,N'-tetrame...		186	C10H22N2O	1000453-48-6	40
4	1-[[2-[Butylamino]butyl]imino]-7...		517	C27H30Cl3N3O	144155-60-2	40
5	3-Pyrazolidinone, 1,4-dimethyl		114	C5H10N2O	006716-36-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031324\
Data File : BM044607.D
Acq On : 13 Mar 2024 21:00
Operator : MA/JU
Sample : P1723-02
Misc :
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Instrument :
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ClientSampleId :
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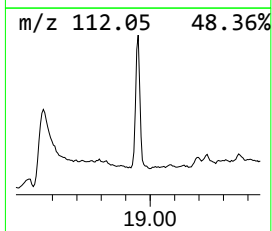
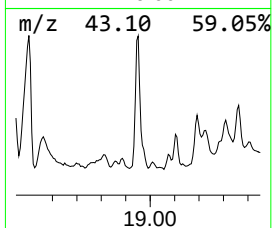
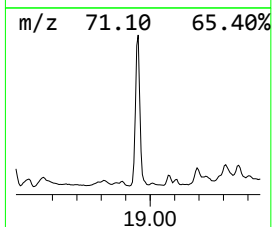
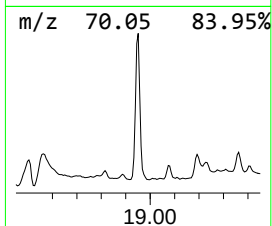
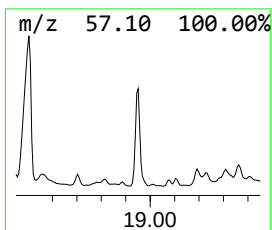
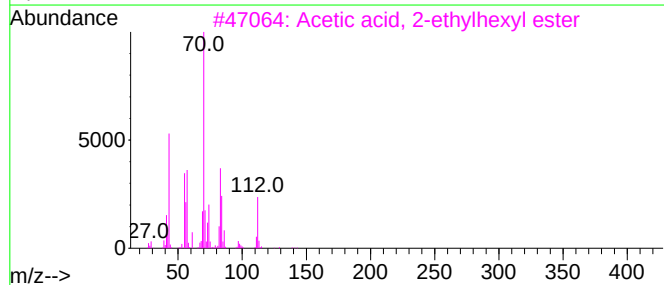
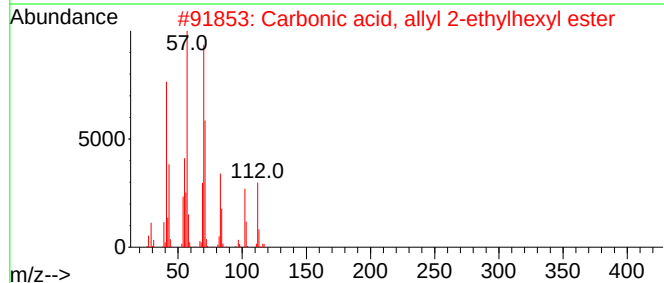
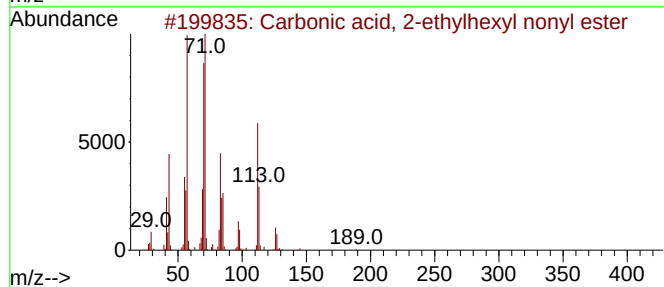
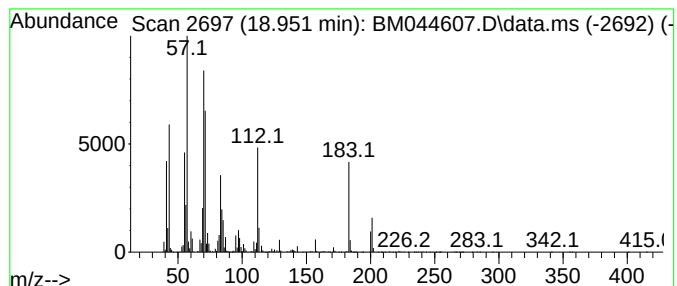
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Carbonic acid, 2-ethylhexyl... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.951	56.70 ng	8685800	Phenanthrene-d10	17.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, 2-ethylhexyl nonyl...	300	C18H36O3	1000383-13-6	53
2			Carbonic acid, allyl 2-ethylhexy...	214	C12H22O3	1000357-80-6	50
3			Acetic acid, 2-ethylhexyl ester	172	C10H20O2	000103-09-3	49
4			Carbonic acid, 2-ethylhexyl unde...	328	C20H40O3	1000383-13-8	46
5			Dodecanoic acid, isooctyl ester	312	C20H40O2	084713-06-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031324\
Data File : BM044607.D
Acq On : 13 Mar 2024 21:00
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Sample : P1723-02
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ClientSampleId :
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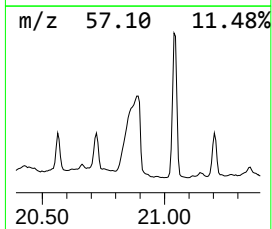
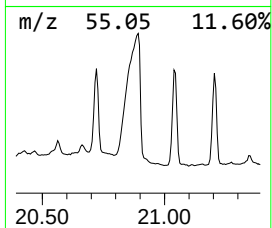
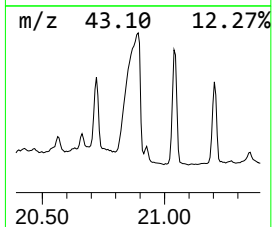
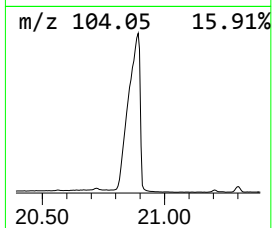
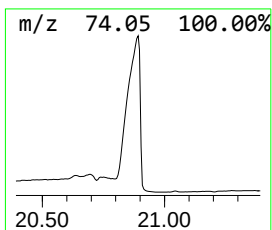
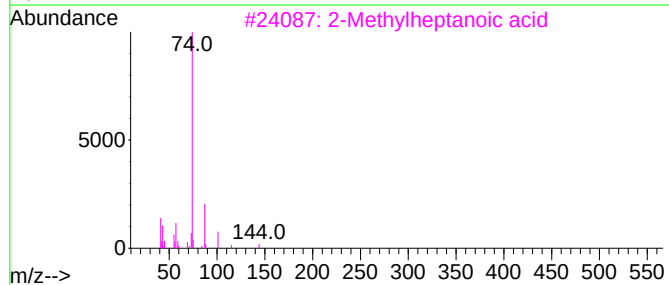
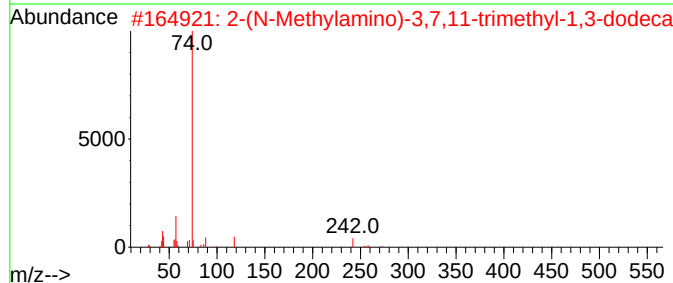
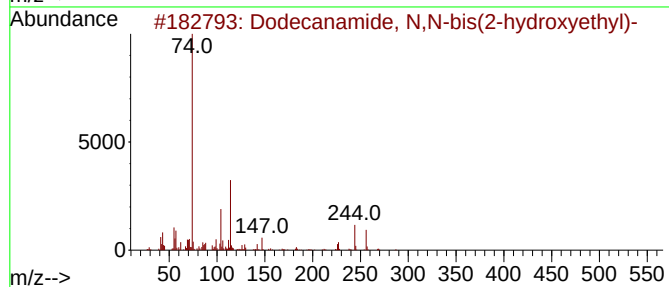
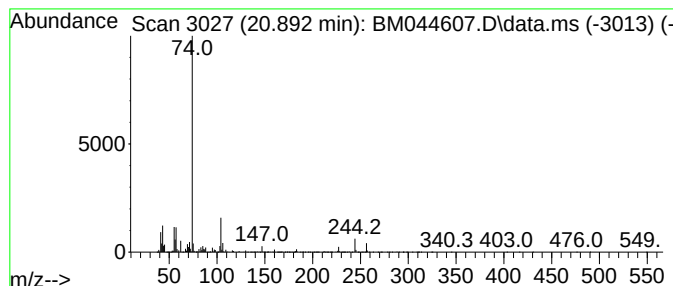
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown20.892 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.892	82.38 ng	51733700	Chrysene-d12	21.303

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanamide, N,N-bis(2-hydroxye...	287	C16H33NO3	000120-40-1	43
2			2-(N-Methylamino)-3,7,11-trimeth...	273	C16H35NO2	1000432-26-9	42
3			2-Methylheptanoic acid	144	C8H16O2	001188-02-9	36
4			1,2,3,4-Undecanetetrol, [2R-(2R*...	220	C11H24O4	137036-71-6	36
5			Dodecanoic acid, 2-methyl-	214	C13H26O2	002874-74-0	36



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031324\
Data File : BM044607.D
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Misc :
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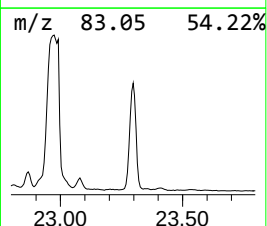
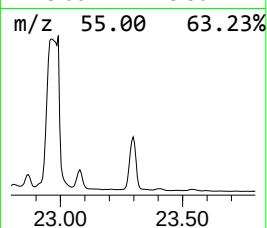
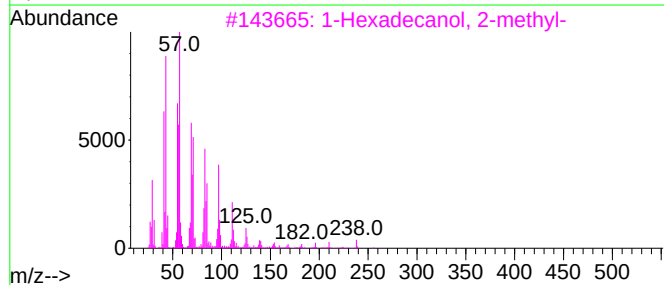
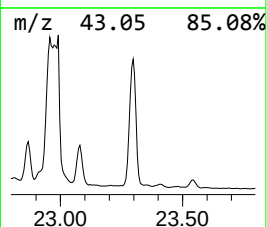
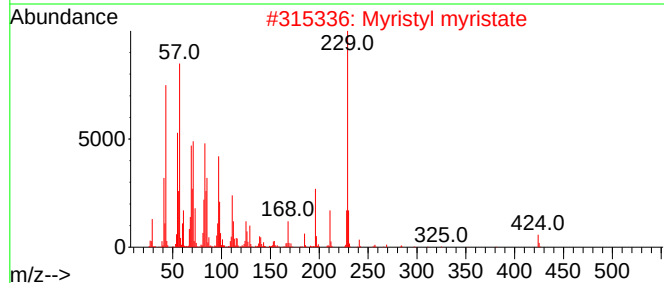
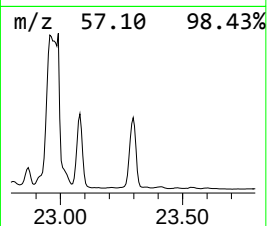
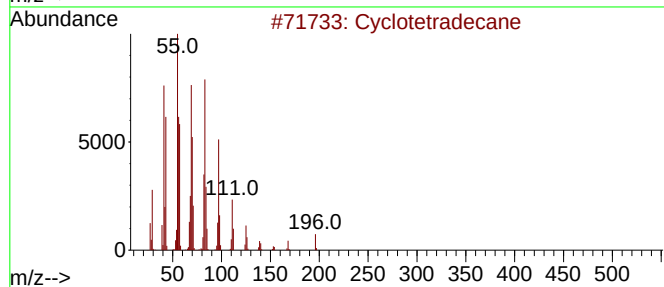
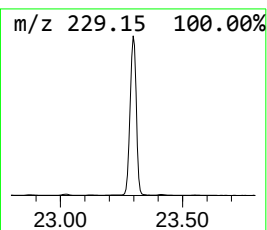
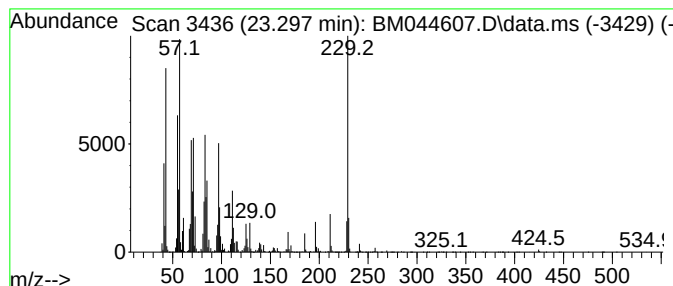
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Cyclotetradecane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.297	74.29 ng	14413300	Perylene-d12	23.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetradecane	196	C14H28	000295-17-0	95
2			Myristyl myristate	424	C28H56O2	003234-85-3	94
3			1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	91
4			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	90
5			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031324\
Data File : BM044607.D
Acq On : 13 Mar 2024 21:00
Operator : MA/JU
Sample : P1723-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

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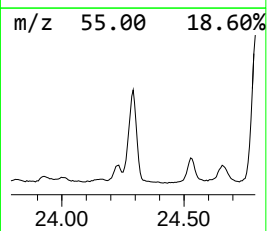
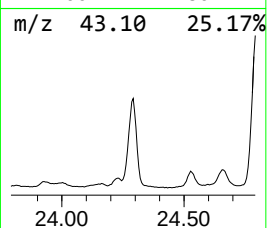
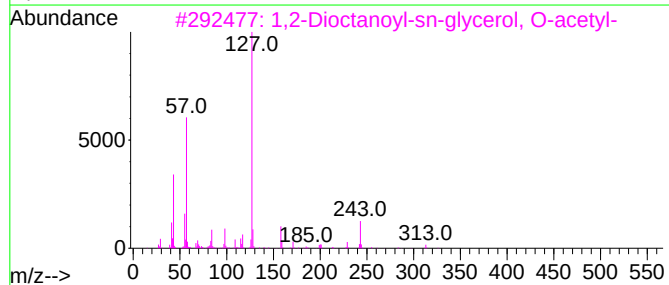
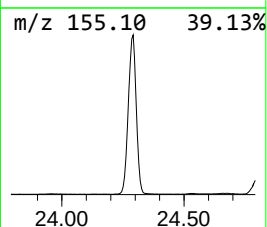
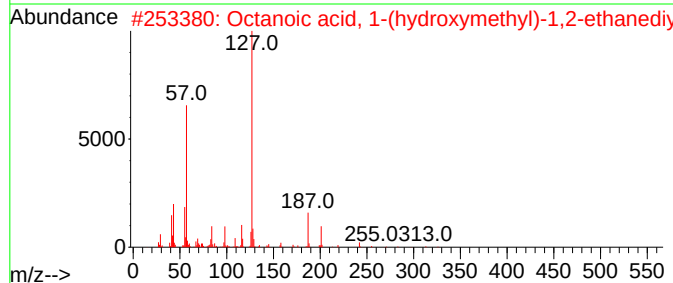
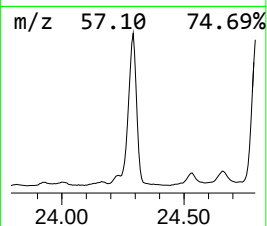
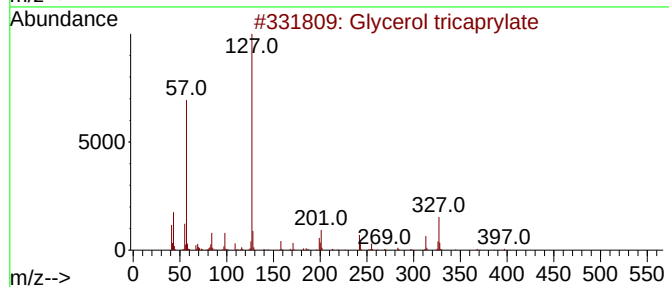
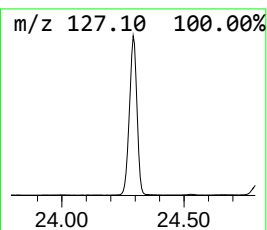
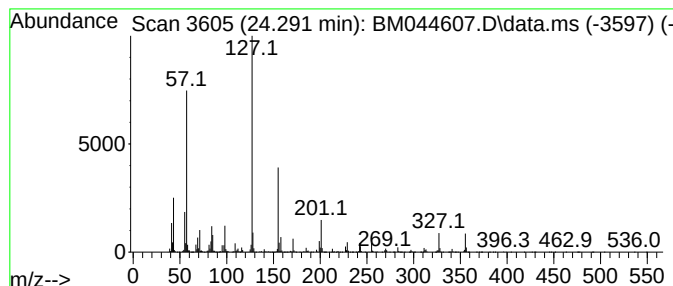
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Glycerol tricaprylate Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.291	68.25 ng	13242300	Perylene-d12	23.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Glycerol tricaprylate	470	C27H50O6	000538-23-8	64
2			Octanoic acid, 1-(hydroxymethyl)...	344	C19H36O5	060514-48-9	53
3			1,2-Dioctanoyl-sn-glycerol, O-ac...	386	C21H38O6	1000452-09-1	50
4			Caprylic anhydride	270	C16H30O3	000623-66-5	50
5			3-Fluoro-5-methoxypyridine	127	C6H6FNO	1060801-62-8	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031324\
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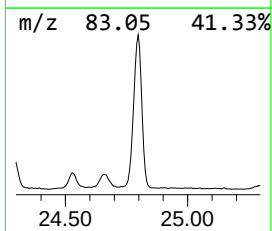
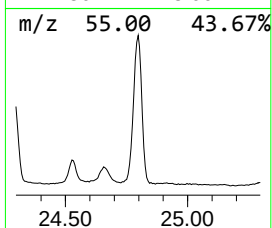
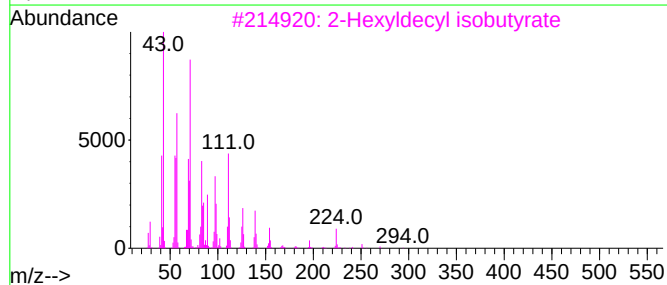
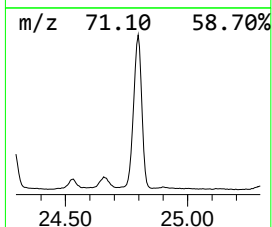
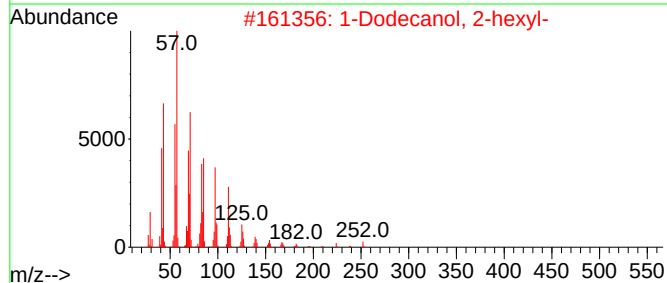
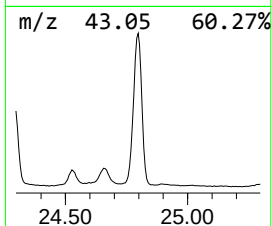
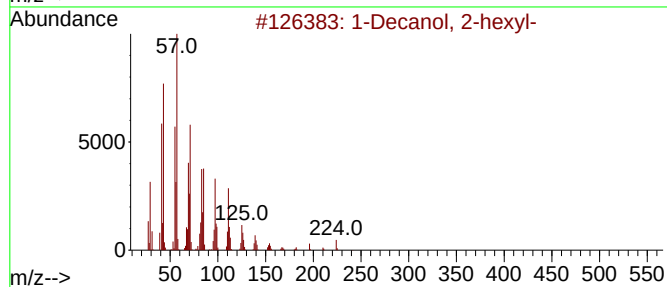
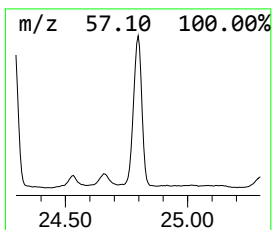
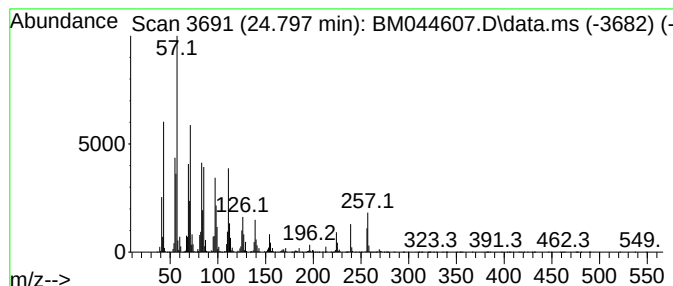
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 1-Decanol, 2-hexyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
24.797	94.20 ng	18275500	Perylene-d12	23.550	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	94
2	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	87
3	2-Hexyldecyl isobutyrate	312	C20H40O2	1000368-55-3	81
4	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	76
5	2-Hexyldecyl acetate	284	C18H36O2	082409-75-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031324\
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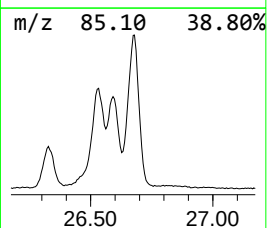
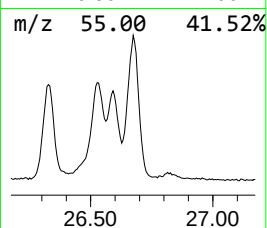
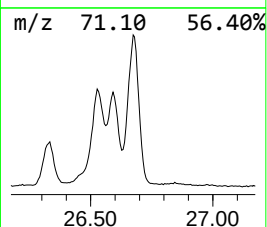
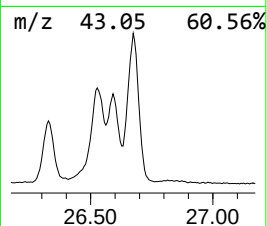
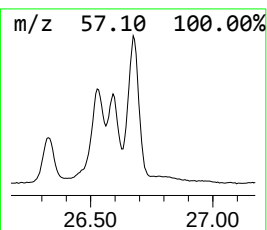
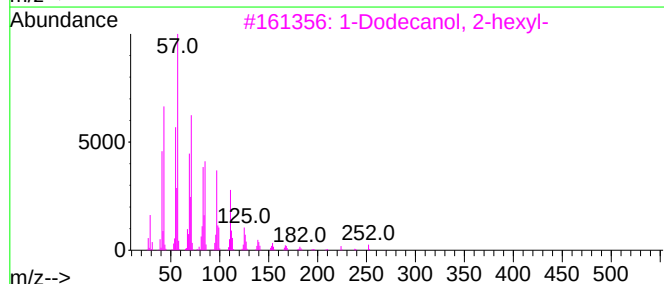
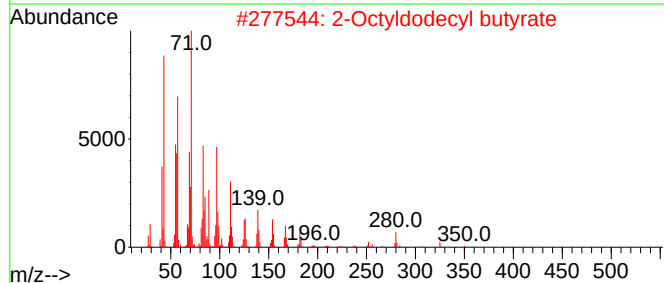
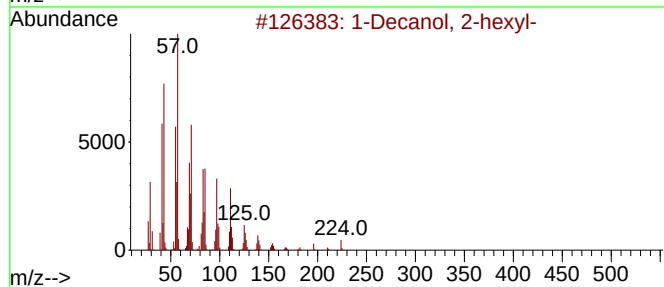
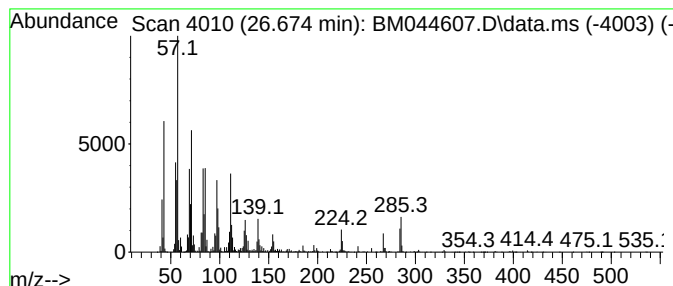
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 2-Octyldodecyl butyrate Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.	
26.674	63.89 ng	12396000	Perylene-d12	23.550	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	91
2	2-Octyldodecyl butyrate	368	C24H48O2	1000368-55-2	90
3	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	81
4	2-Hexyldodecyl isobutyrate	312	C20H40O2	1000368-55-3	76
5	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031324\
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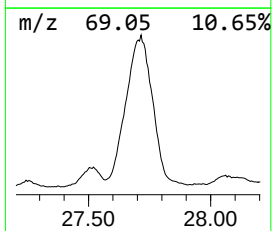
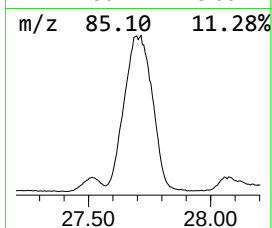
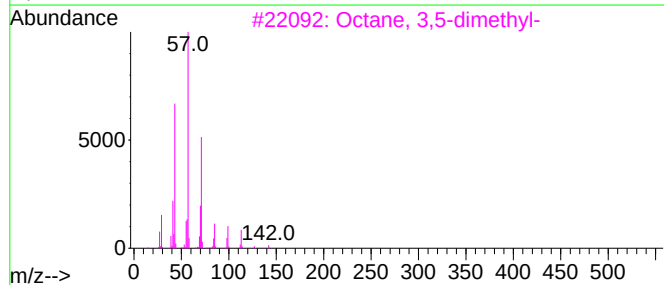
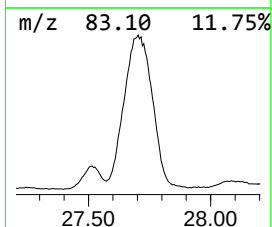
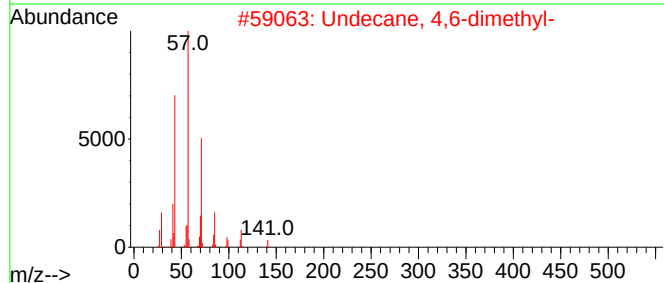
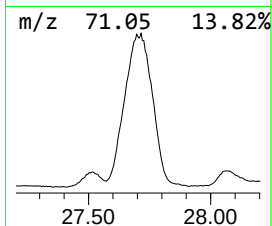
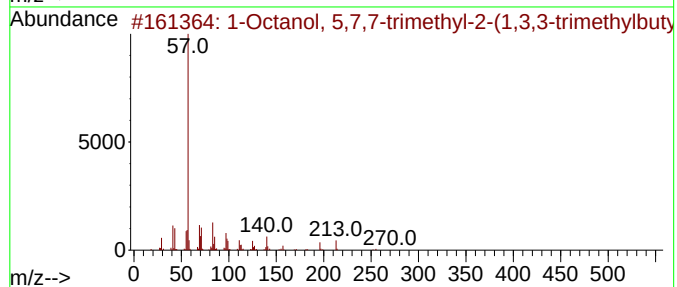
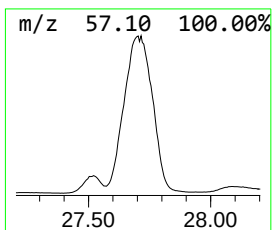
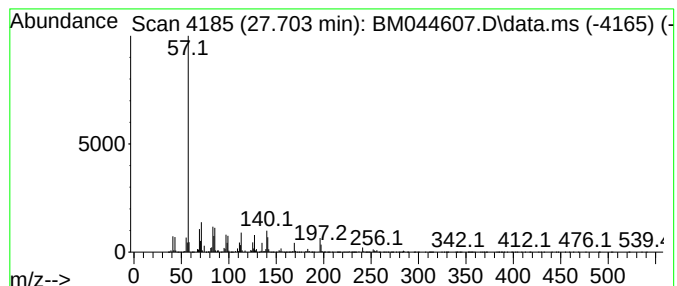
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown27.703 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.703	138.01 ng	26775800	Perylene-d12	23.550

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Octanol, 5,7,7-trimethyl-2-(1,...	270	C18H38O	036400-98-3	50
2		Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	46
3		Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	43
4		Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	38
5		Carbonic acid, decyl dodecyl ester	370	C23H46O3	1000383-16-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031324\
Data File : BM044607.D
Acq On : 13 Mar 2024 21:00
Operator : MA/JU
Sample : P1723-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EFF-WW

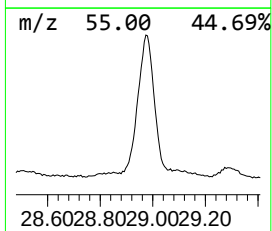
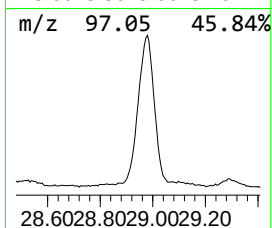
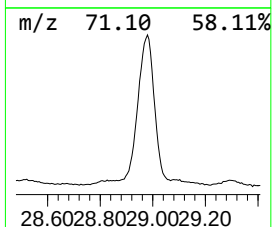
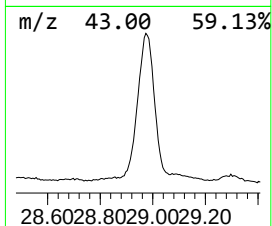
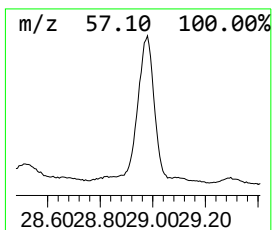
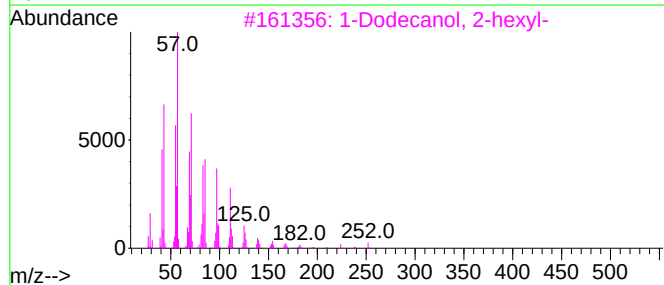
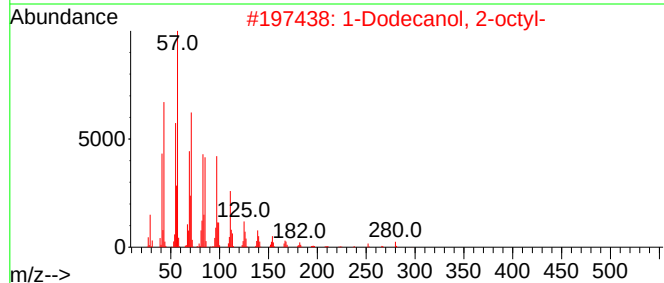
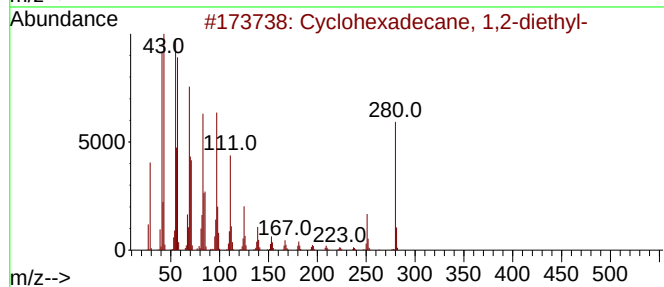
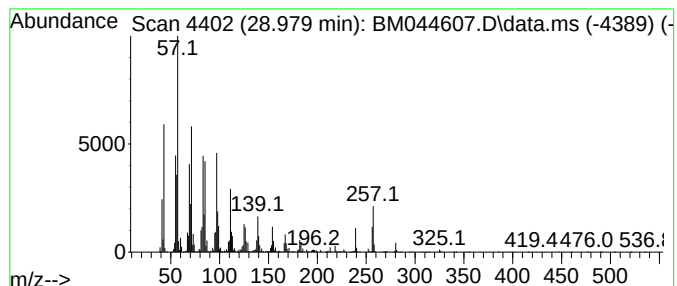
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Cyclohexadecane, 1,2-diethyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.979	54.93 ng	10656500	Perylene-d12	23.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	90
2			1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	81
3			1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	76
4			1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	76
5			Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031324\
Data File : BM044607.D
Acq On : 13 Mar 2024 21:00
Operator : MA/JU
Sample : P1723-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EFF-WW

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.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
Hexanoic acid, ...	9.316	222.4	ng	32855400	2	10.510	2954800	20.0
Octanoic acid	10.210	455.9	ng	67349700	2	10.510	2954800	20.0
n-Decanoic acid	12.828	434.1	ng	62912100	3	14.351	2898510	20.0
Dodecanoic acid	15.051	1584.0	ng	229566000	3	14.351	2898510	20.0
1-Octanol, 5,7,...	16.286	143.6	ng	22001200	4	17.104	3063700	20.0
Trifluoroacetic...	16.333	246.6	ng	37780900	4	17.104	3063700	20.0
Carbonic acid, ...	16.386	171.2	ng	26230800	4	17.104	3063700	20.0
Tetradecanoic acid	16.586	286.4	ng	43867100	4	17.104	3063700	20.0
n-Hexadecanoic ...	18.027	96.6	ng	14803400	4	17.104	3063700	20.0
Methyl valerate	18.504	130.5	ng	19988300	4	17.104	3063700	20.0
Oxazolidine, 3-...	18.562	83.7	ng	12819300	4	17.104	3063700	20.0
Carbonic acid, ...	18.951	56.7	ng	8685800	4	17.104	3063700	20.0
unknown20.892	20.892	82.4	ng	51733700	5	21.303	12559400	20.0
4-Hydrazono-5-h...	22.974	243.0	ng	47153600	6	23.550	3880270	20.0
Cyclotetradecane	23.297	74.3	ng	14413300	6	23.550	3880270	20.0
Glycerol tricap...	24.291	68.3	ng	13242300	6	23.550	3880270	20.0
1-Decanol, 2-he...	24.797	94.2	ng	18275500	6	23.550	3880270	20.0
2-Octyldodecyl ...	26.674	63.9	ng	12396000	6	23.550	3880270	20.0
unknown27.703	27.703	138.0	ng	26775800	6	23.550	3880270	20.0
Cyclohexadecane...	28.979	54.9	ng	10656500	6	23.550	3880270	20.0