

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
 Data File : BG057906.D
 Acq On : 29 Jun 2023 16:03
 Operator : CG/JU
 Sample : 03324-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 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_G\Methods\8270-BG062723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057906.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.175	179	185	200	rVB	1106694	1828009	2.77%	0.395%
2	4.422	221	227	232	rBV	522762	823180	1.25%	0.178%
3	4.551	242	249	261	rVB	428734	679041	1.03%	0.147%
4	5.027	318	330	339	rVB	963507	1582459	2.40%	0.342%
5	5.497	402	410	416	rBV	354266	910637	1.38%	0.197%
6	7.306	709	718	723	rVB3	240487	811297	1.23%	0.175%
7	7.912	808	821	826	rBV3	266593	702136	1.06%	0.152%
8	8.100	826	853	857	rBV3	10225238	66043466	100.00%	14.268%
9	9.087	1012	1021	1028	rBV2	871553	1581106	2.39%	0.342%
10	9.439	1039	1081	1084	rBV	855380	6140172	9.30%	1.326%
11	9.480	1084	1088	1100	rVB	450760	716568	1.08%	0.155%
12	10.420	1181	1248	1249	rBV2	1681033	18754950	28.40%	4.052%
13	13.082	1654	1701	1704	rBV	3181125	24270732	36.75%	5.243%
14	13.176	1711	1717	1722	rBV	1523098	2412853	3.65%	0.521%
15	14.192	1885	1890	1899	rVB2	1240000	1776049	2.69%	0.384%
16	14.445	1922	1933	1939	rBV	460452	893469	1.35%	0.193%
17	14.545	1945	1950	1961	rVB2	554645	1172043	1.77%	0.253%
18	14.662	1965	1970	1979	rVB	669870	888747	1.35%	0.192%
19	15.197	2019	2061	2063	rBV2	7384683	53409564	80.87%	11.538%
20	15.890	2173	2179	2188	rVB	4355202	6053084	9.17%	1.308%
21	15.990	2191	2196	2201	rVV	587666	800398	1.21%	0.173%
22	16.049	2201	2206	2211	rVV2	894913	1409397	2.13%	0.304%
23	16.102	2211	2215	2221	rVB	1842051	2342318	3.55%	0.506%
24	16.478	2271	2279	2283	rBV	2292243	3479897	5.27%	0.752%
25	16.531	2283	2288	2292	rVV	4354934	6893634	10.44%	1.489%
26	16.578	2292	2296	2307	rVB	3092305	4783502	7.24%	1.033%
27	16.872	2319	2346	2350	rBV	8239892	45767519	69.30%	9.887%
28	16.936	2352	2357	2364	rVB	1316545	2567602	3.89%	0.555%
29	17.077	2377	2381	2393	rVB	535141	952067	1.44%	0.206%
30	17.301	2414	2419	2425	rBV	585642	894243	1.35%	0.193%
31	17.800	2497	2504	2518	rVB3	311410	705670	1.07%	0.152%
32	17.918	2520	2524	2529	rBV	610403	795492	1.20%	0.172%
33	18.105	2547	2556	2566	rBV5	296085	1036283	1.57%	0.224%
34	18.288	2567	2587	2590	rBV	7520046	28851356	43.69%	6.233%
35	18.505	2618	2624	2632	rVB2	478952	985721	1.49%	0.213%
36	18.617	2639	2643	2648	rVB	982937	1299725	1.97%	0.281%

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37	19.122	2724	2729	2737	rBV	3981990	5791120	8.77%	1.251%
38	19.245	2746	2750	2754	rBV	1192088	1387541	2.10%	0.300%
39	19.404	2762	2777	2782	rBV	5588761	15603902	23.63%	3.371%
40	19.451	2782	2785	2788	rVV	967458	1602150	2.43%	0.346%
41	19.492	2789	2792	2795	rVV	1405498	1988502	3.01%	0.430%
42	19.522	2795	2797	2803	rVB3	844607	1156985	1.75%	0.250%
43	19.651	2815	2819	2822	rBV	1030866	1136821	1.72%	0.246%
44	19.704	2824	2828	2832	rVB	1363979	1677240	2.54%	0.362%
45	19.815	2841	2847	2854	rVB	4463673	6290181	9.52%	1.359%
46	19.921	2860	2865	2870	rVB	2347091	3208235	4.86%	0.693%
47	19.974	2870	2874	2878	rBV	714321	832404	1.26%	0.180%
48	20.191	2907	2911	2913	rBV	580456	710729	1.08%	0.154%
49	20.221	2913	2916	2921	rVB	2243557	2664531	4.03%	0.576%
50	20.362	2935	2940	2944	rVB	5240396	6923543	10.48%	1.496%
51	20.503	2959	2964	2968	rVB2	693313	1000046	1.51%	0.216%
52	20.708	2995	2999	3005	rVB	895063	1237981	1.87%	0.267%
53	20.879	3022	3028	3031	rBV	4621192	6349667	9.61%	1.372%
54	20.914	3031	3034	3040	rVB	672601	747441	1.13%	0.161%
55	20.984	3041	3046	3049	rBV	605938	936967	1.42%	0.202%
56	21.225	3080	3087	3092	rVB	7242983	11458243	17.35%	2.475%
57	21.413	3113	3119	3126	rBV	4189151	6073099	9.20%	1.312%
58	21.554	3139	3143	3146	rBV	504497	866767	1.31%	0.187%
59	21.936	3203	3208	3216	rBV2	432460	1436371	2.17%	0.310%
60	22.218	3250	3256	3261	rVV	1670136	2956435	4.48%	0.639%
61	22.271	3261	3265	3272	rVV2	812978	1713108	2.59%	0.370%
62	22.371	3272	3282	3287	rVB	7955400	16532582	25.03%	3.572%
63	22.671	3328	3333	3347	rVB	357242	1155884	1.75%	0.250%
64	23.740	3508	3515	3523	rBV2	1379063	3003963	4.55%	0.649%
65	23.975	3524	3555	3570	rVB4	10556849	59005857	89.34%	12.747%
66	24.715	3675	3681	3695	rVB2	323228	915850	1.39%	0.198%
67	26.977	4059	4066	4082	rVB2	464876	1512873	2.29%	0.327%

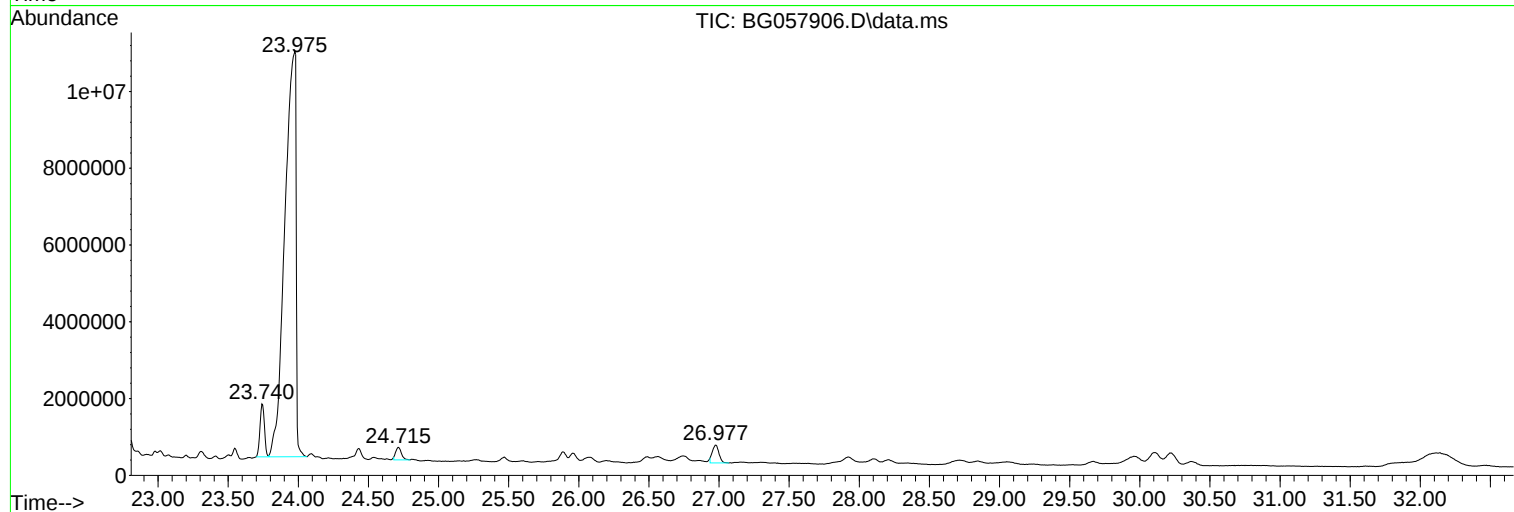
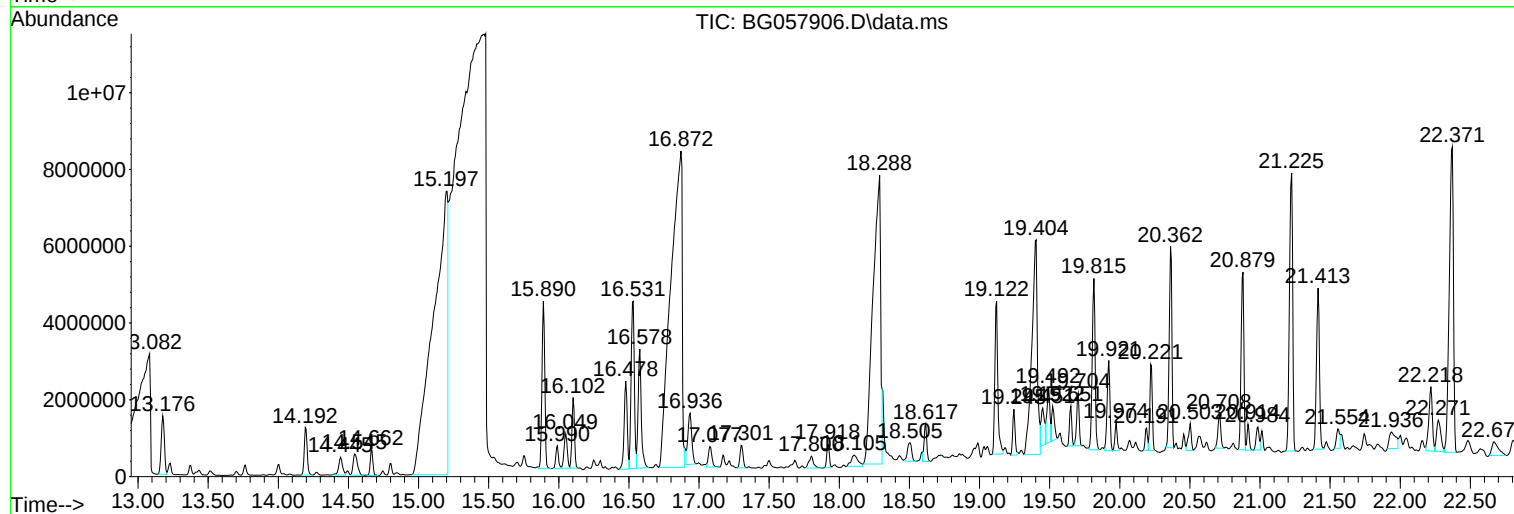
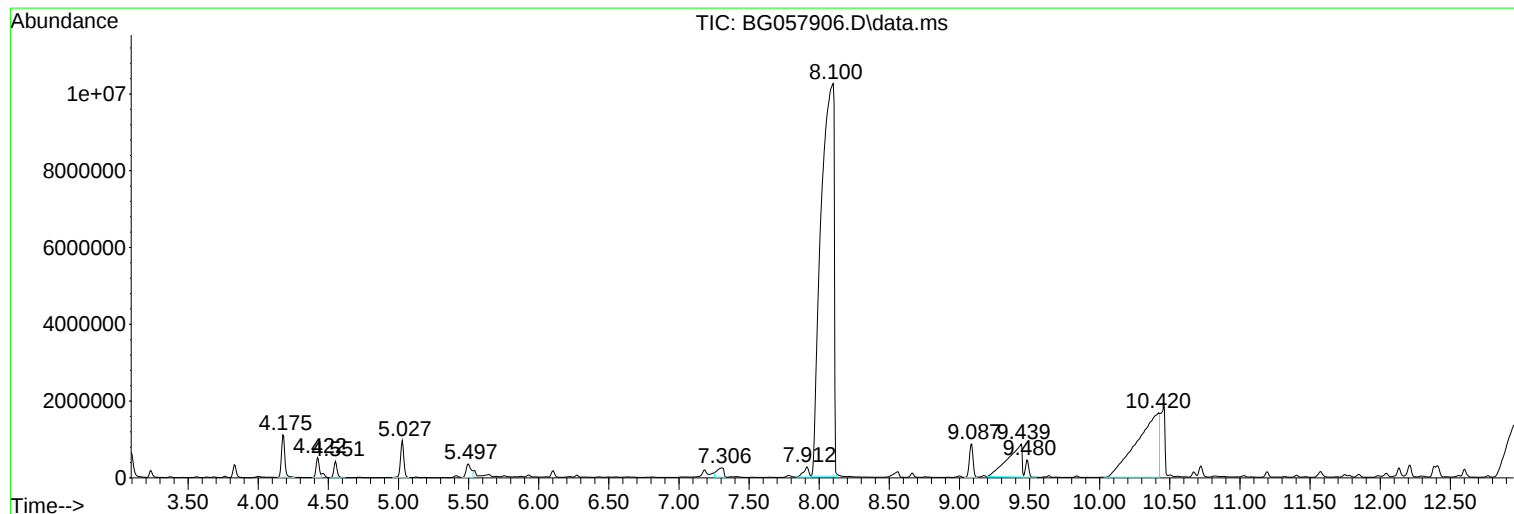
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BNA_G
ClientSampleId :
EFF-WW

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.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 :
BNA_G
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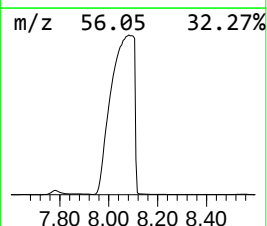
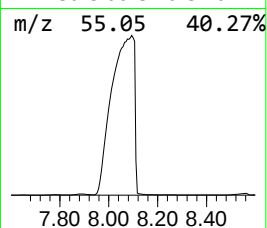
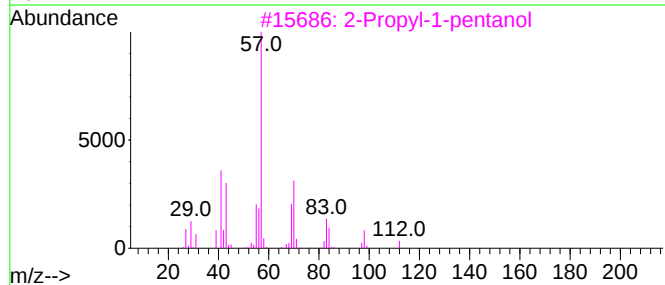
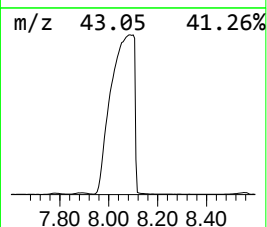
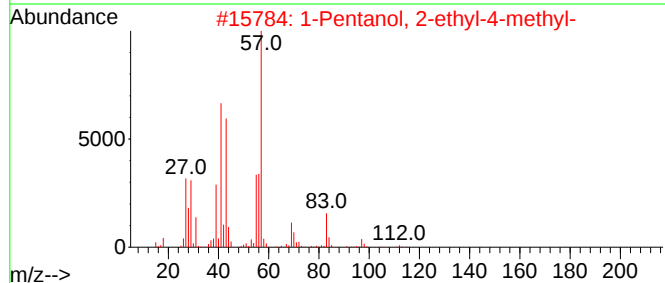
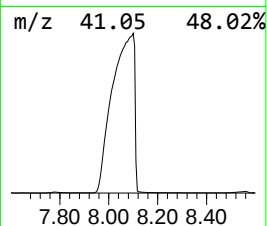
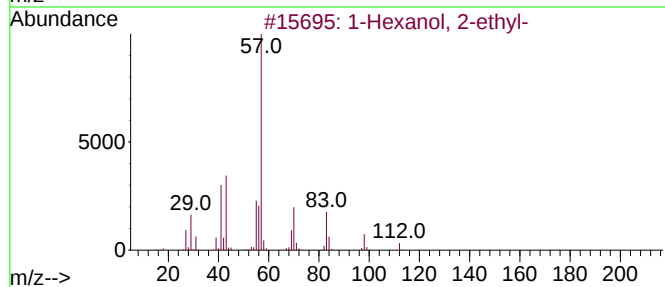
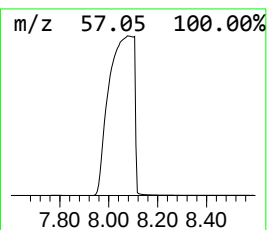
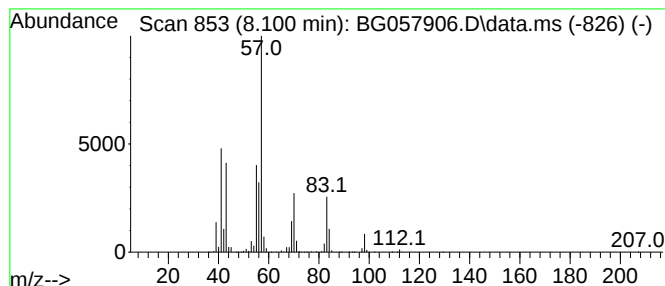
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.100	1881.22 ng	66043500	1,4-Dichlorobenzene-d4	7.917

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	83
2	1-Pentanol, 2-ethyl-4-methyl-			130	C8H18O	000106-67-2	59
3	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	59
4	Pentadecafluorooctanoic acid, 2-...			526	C16H17F15O2	1000406-80-9	53
5	Heptane, 1,1'-oxybis-			214	C14H30O	000629-64-1	47



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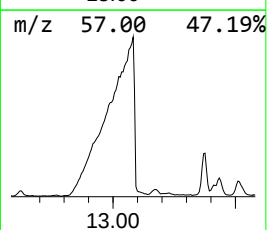
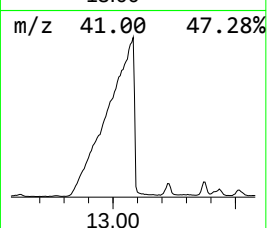
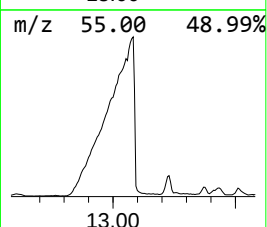
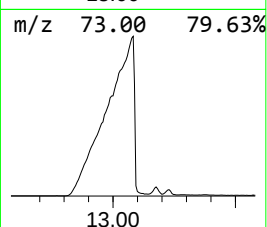
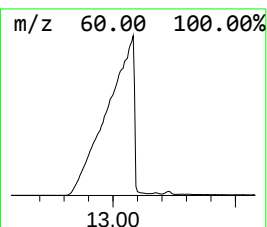
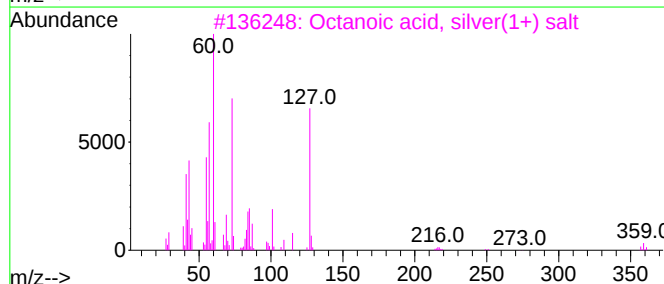
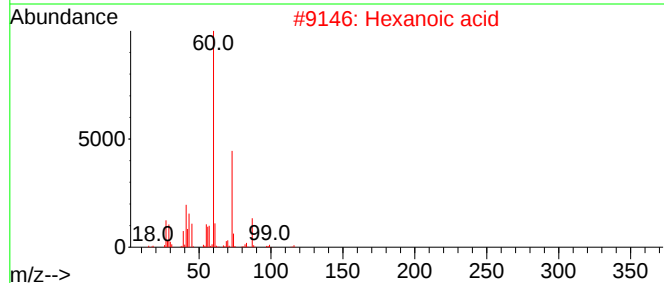
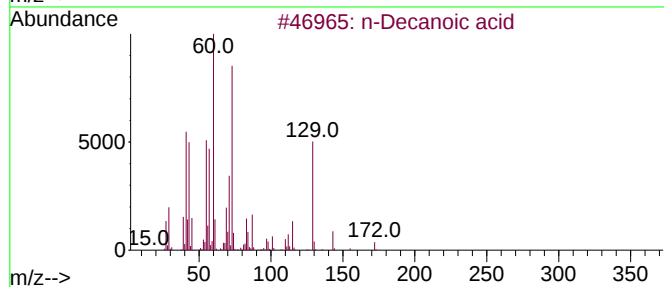
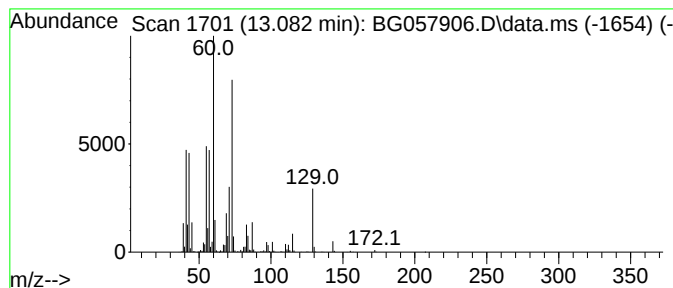
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Decanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.082	414.16 ng	24270700	Acenaphthene-d10	14.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Decanoic acid	172	C10H20O2	000334-48-5	97
2			Hexanoic acid	116	C6H12O2	000142-62-1	52
3			Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	52
4			Heptanoic acid	130	C7H14O2	000111-14-8	50
5			Nonanoic acid	158	C9H18O2	000112-05-0	45



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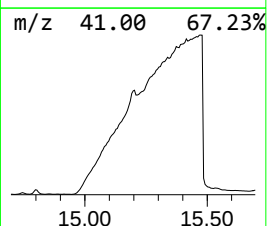
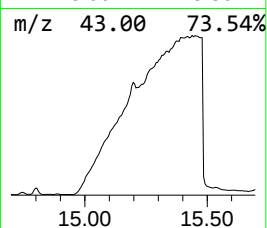
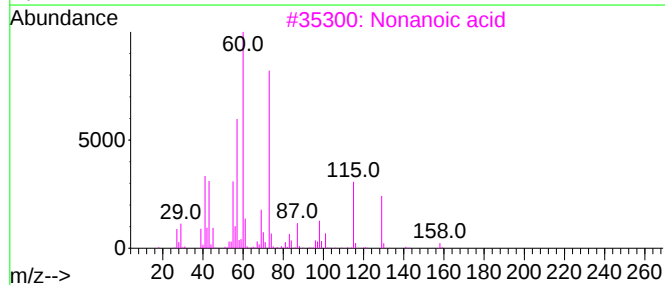
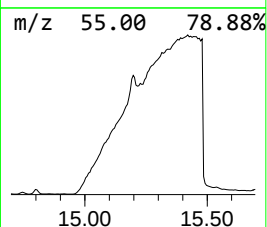
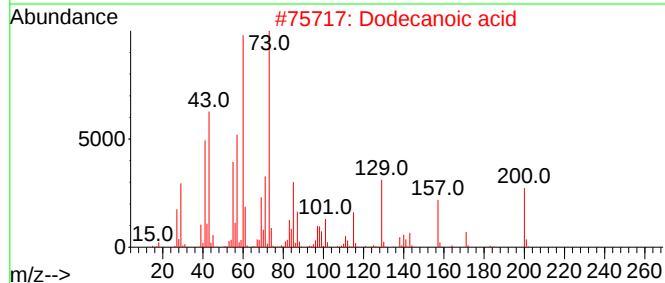
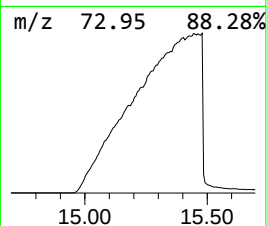
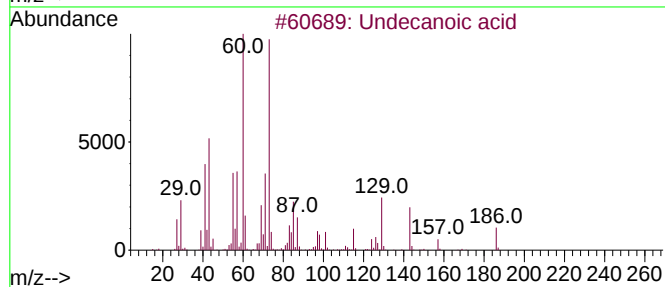
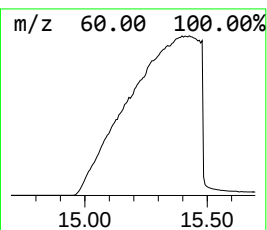
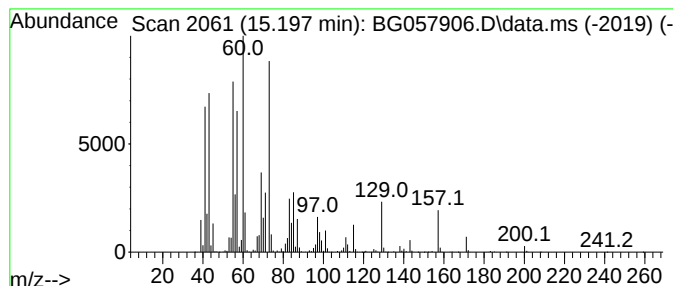
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Undecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.197	911.39 ng	53409600	Acenaphthene-d10	14.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecanoic acid	186	C11H22O2	000112-37-8	72
2			Dodecanoic acid	200	C12H24O2	000143-07-7	72
3			Nonanoic acid	158	C9H18O2	000112-05-0	70
4			Octanoic acid	144	C8H16O2	000124-07-2	49
5			.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	38



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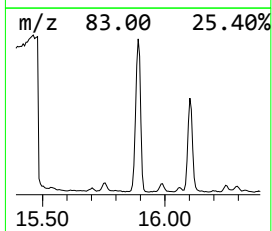
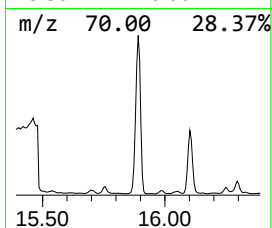
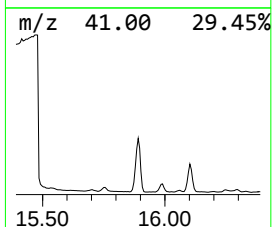
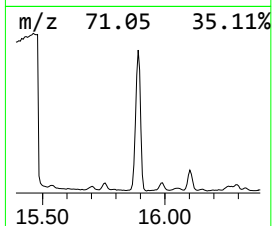
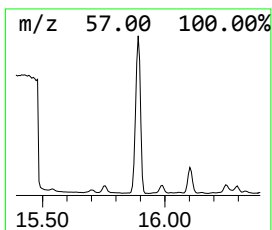
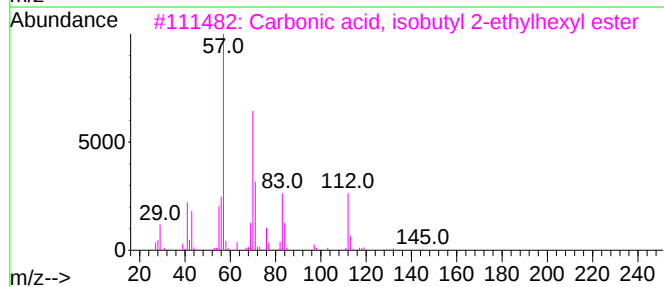
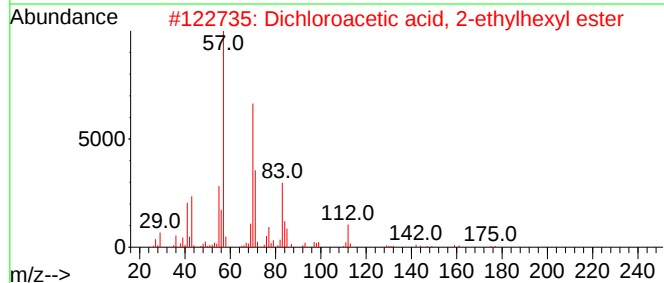
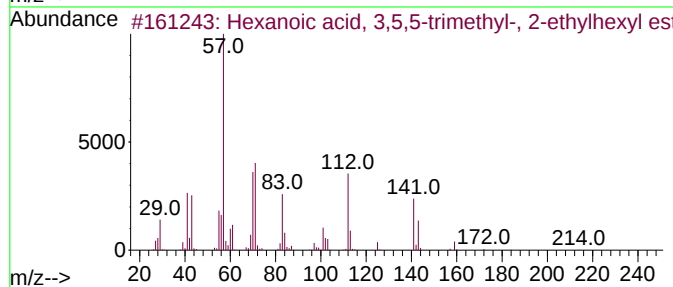
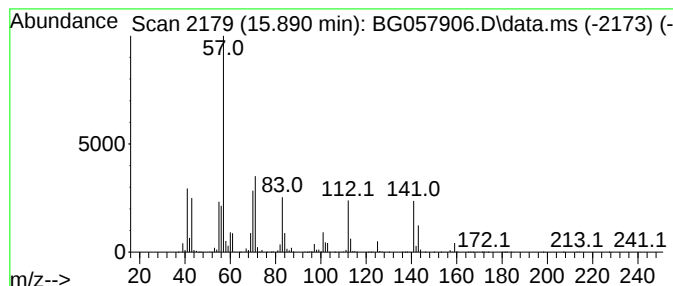
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexanoic acid, 3,5,5-trimet... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.890	103.29 ng	6053080	Acenaphthene-d10	14.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 3,5,5-trimethyl-,...	270	C17H34O2	1000406-82-2	91
2			Dichloroacetic acid, 2-ethylhexy...	240	C10H18Cl2O2	068144-72-9	43
3			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	43
4			Hexanoic acid, 3,5,5-trimethyl-,...	214	C13H26O2	1000406-05-3	38
5			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
Data File : BG057906.D
Acq On : 29 Jun 2023 16:03
Operator : CG/JU
Sample : 03324-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EFF-WW

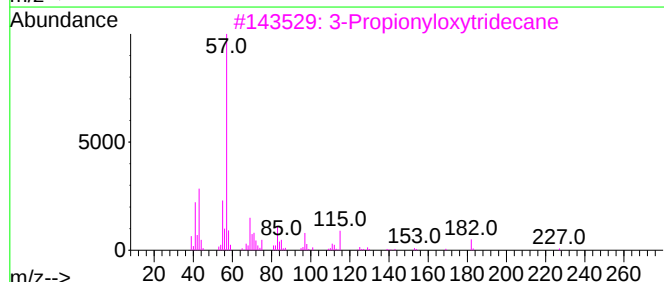
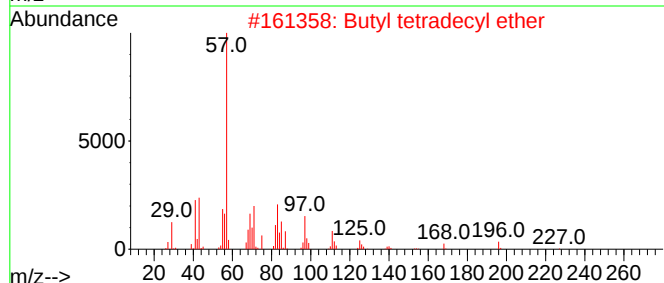
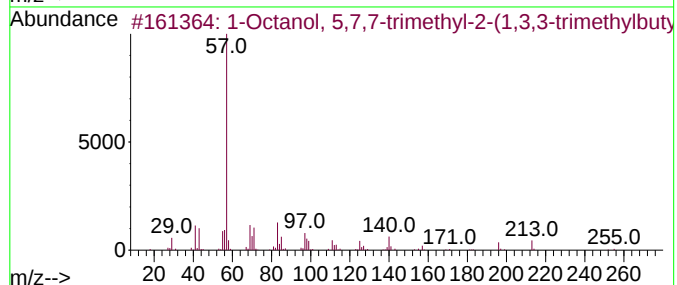
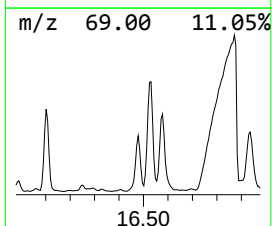
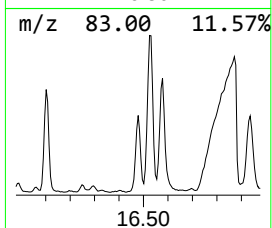
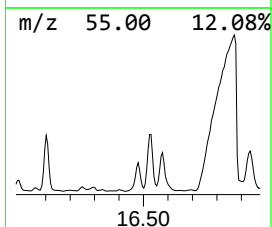
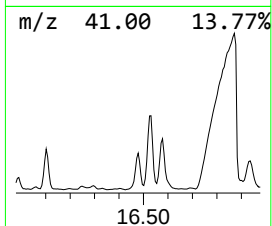
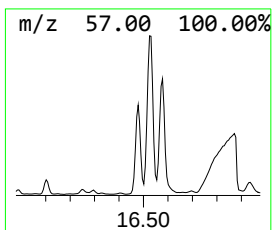
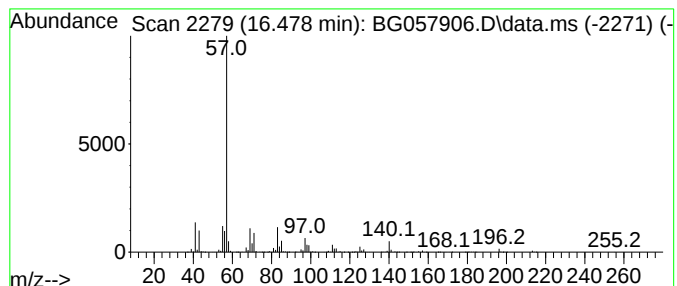
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Octanol, 5,7,7-trimethyl-... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.478	77.83 ng	3479900	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	72
2			Butyl tetradecyl ether	270	C18H38O	1000406-40-4	53
3			3-Propionyloxytridecane	256	C16H32O2	1000245-62-5	53
4			Pentadecafluorooctanoic acid, te...	610	C22H29F15O2	1000406-04-4	53
5			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
Data File : BG057906.D
Acq On : 29 Jun 2023 16:03
Operator : CG/JU
Sample : 03324-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EFF-WW

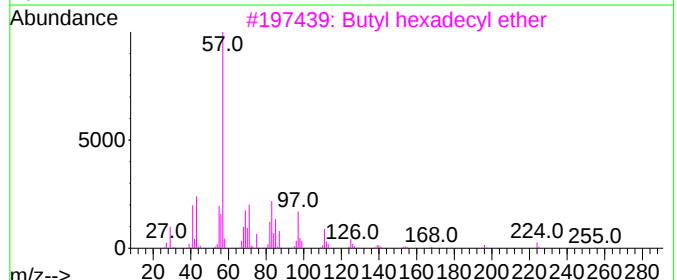
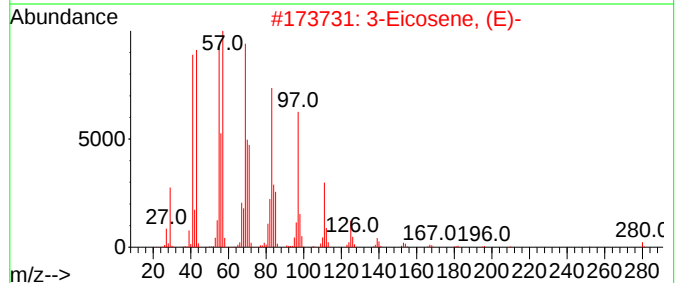
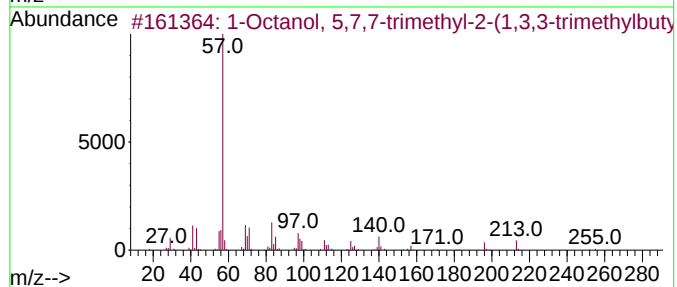
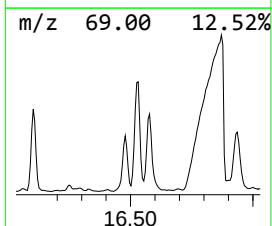
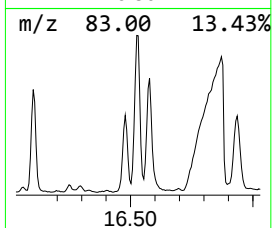
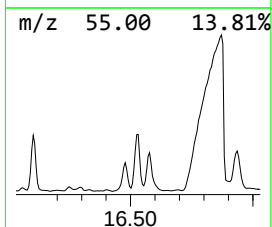
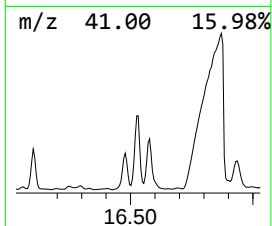
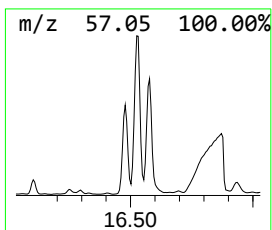
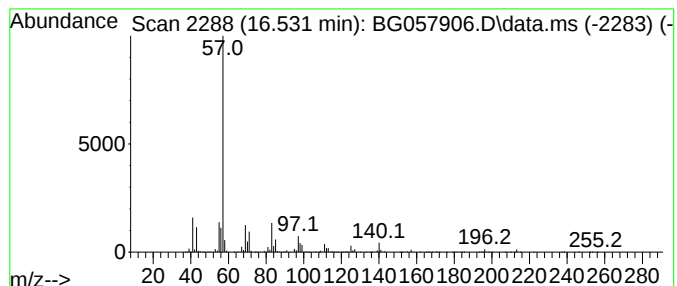
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 3-Eicosene, (E)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.531	154.18 ng	6893630	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	91
2			3-Eicosene, (E)-	280	C20H40	074685-33-9	59
3			Butyl hexadecyl ether	298	C20H42O	1010406-40-5	59
4			Trichloroacetic acid, undecyl ester	316	C13H23Cl3O2	074339-49-4	53
5			3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
Data File : BG057906.D
Acq On : 29 Jun 2023 16:03
Operator : CG/JU
Sample : 03324-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

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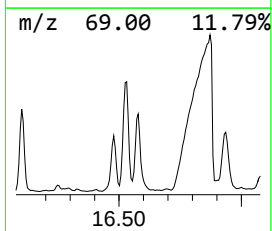
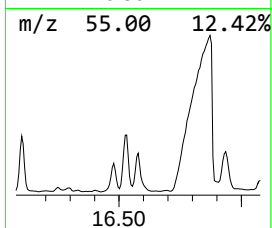
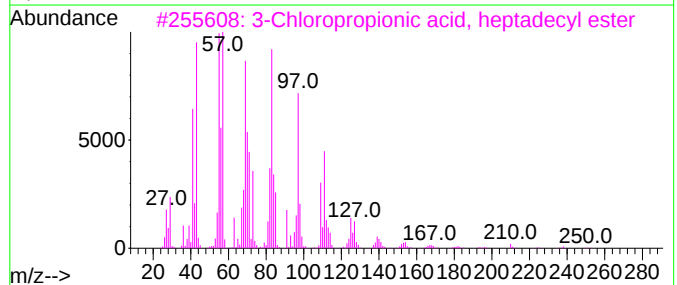
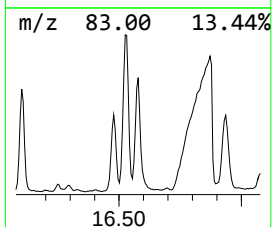
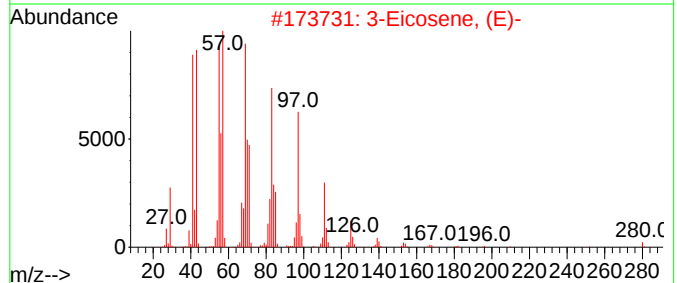
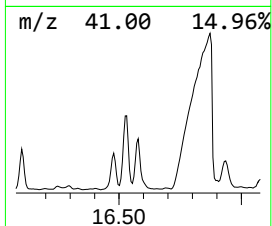
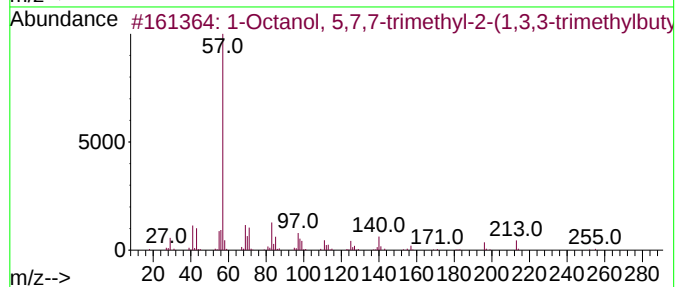
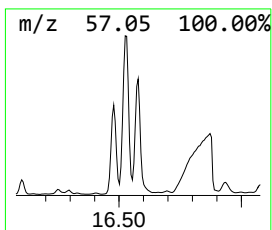
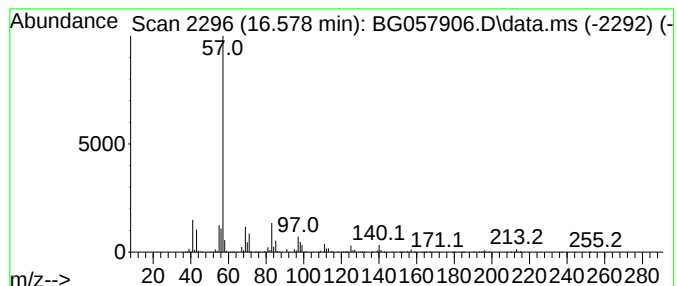
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 3-Chloropropionic acid, hep... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.578	106.98 ng	4783500	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	90		
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	59		
3	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	53		
4	Trichloroacetic acid, undecyl ester	316	C13H23Cl3O2	074339-49-4	53		
5	1-Dodecanol, 3,7,11-trimethyl-	228	C15H32O	006750-34-1	53		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
Data File : BG057906.D
Acq On : 29 Jun 2023 16:03
Operator : CG/JU
Sample : 03324-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EFF-WW

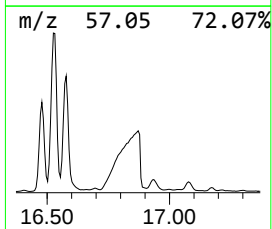
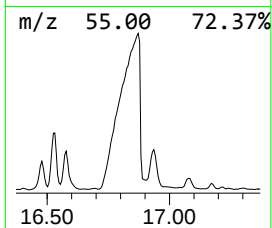
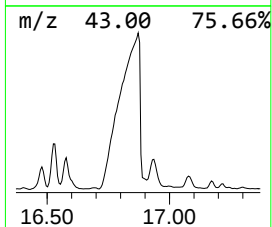
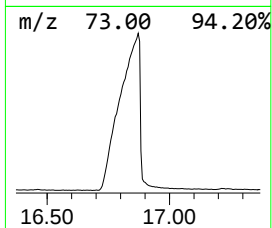
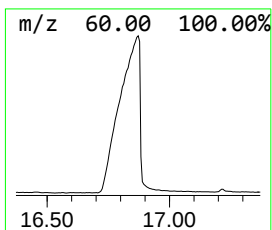
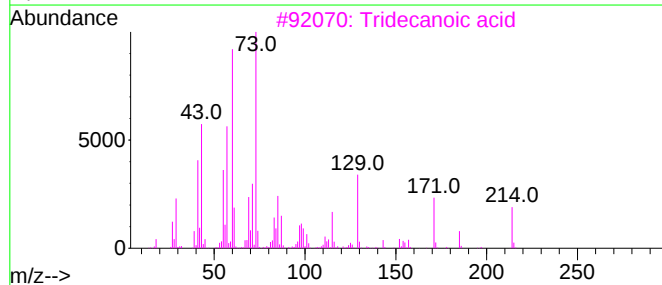
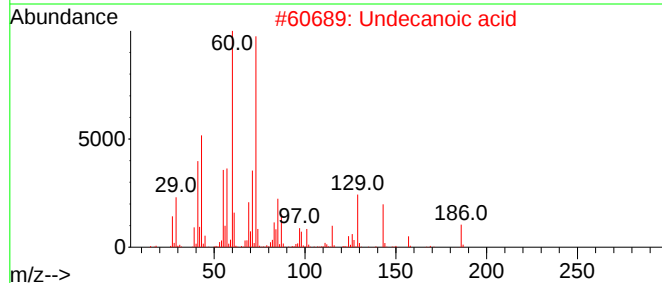
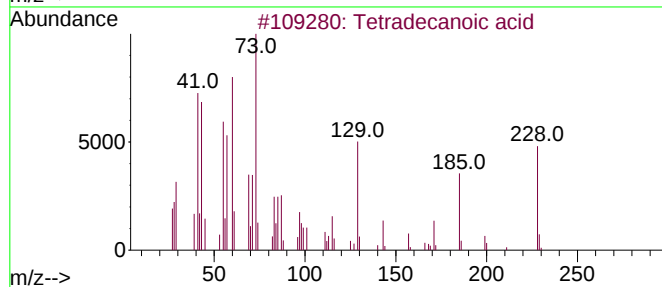
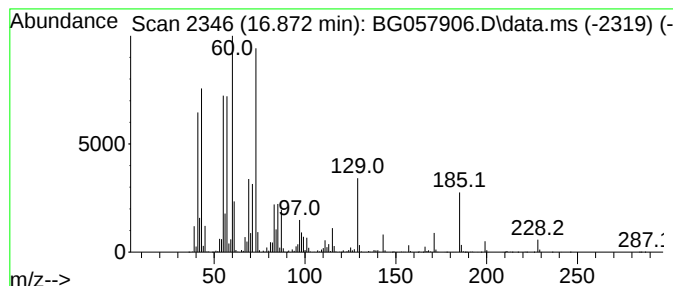
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetradecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.872	1023.60 ng	45767500	Phenanthrene-d10	17.307

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	96
2			Undecanoic acid	186	C11H22O2	000112-37-8	76
3			Tridecanoic acid	214	C13H26O2	000638-53-9	72
4			Dodecanoic acid	200	C12H24O2	000143-07-7	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
Data File : BG057906.D
Acq On : 29 Jun 2023 16:03
Operator : CG/JU
Sample : 03324-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

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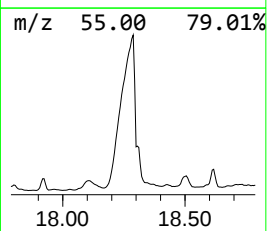
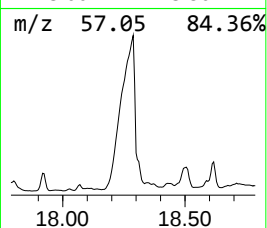
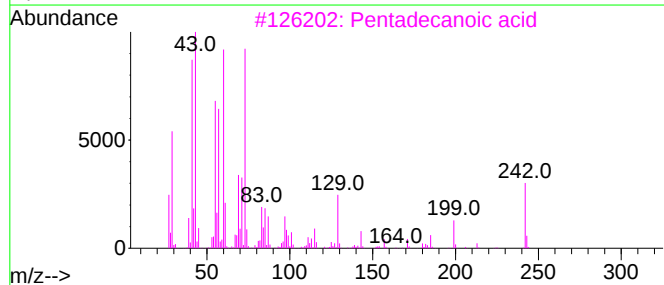
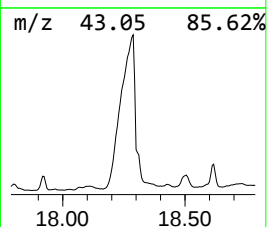
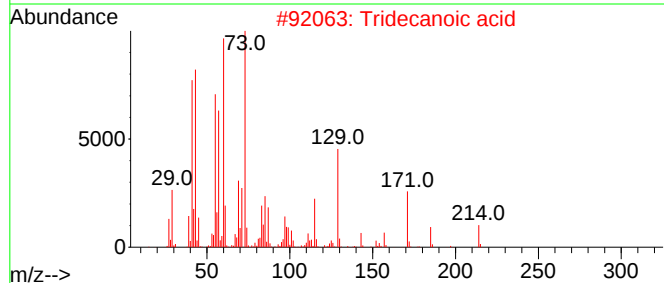
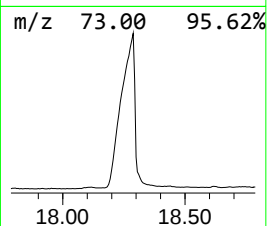
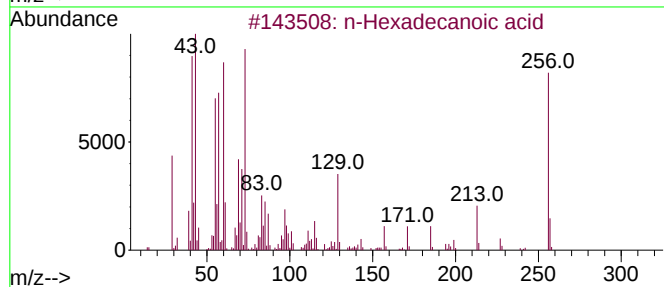
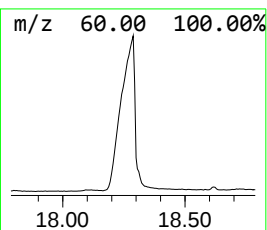
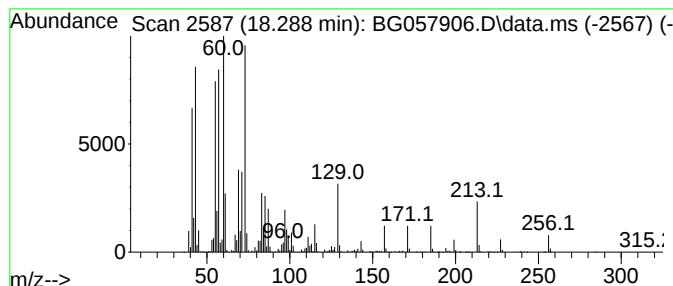
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.288	645.27 ng	28851400	Phenanthrene-d10	17.307

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Dodecanoic acid	200	C12H24O2	000143-07-7	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
Data File : BG057906.D
Acq On : 29 Jun 2023 16:03
Operator : CG/JU
Sample : 03324-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

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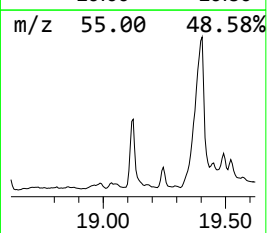
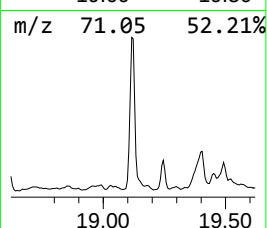
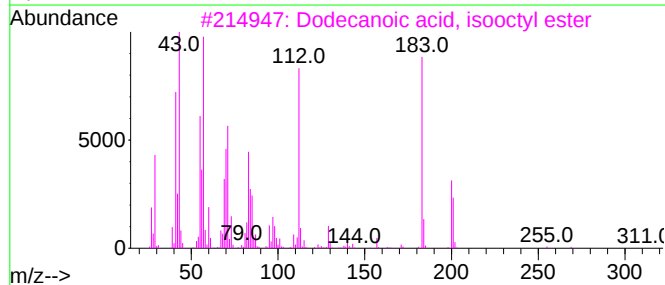
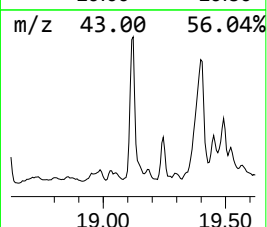
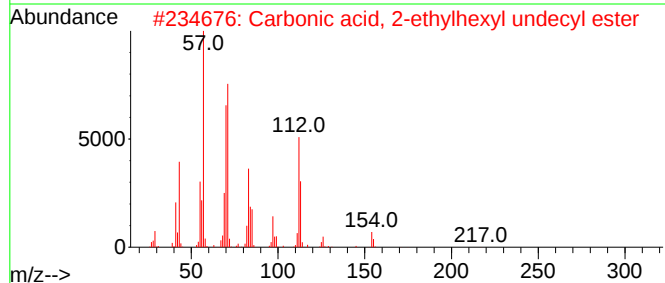
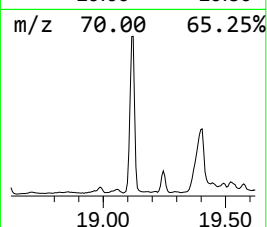
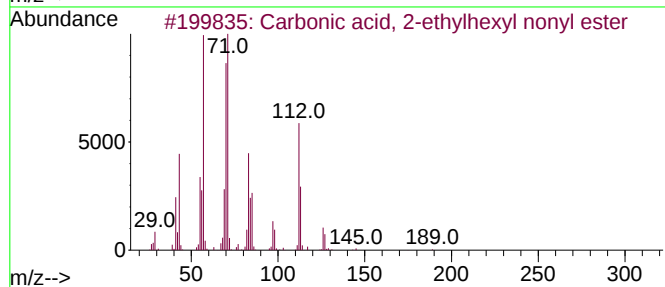
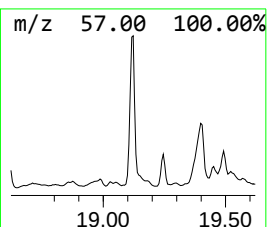
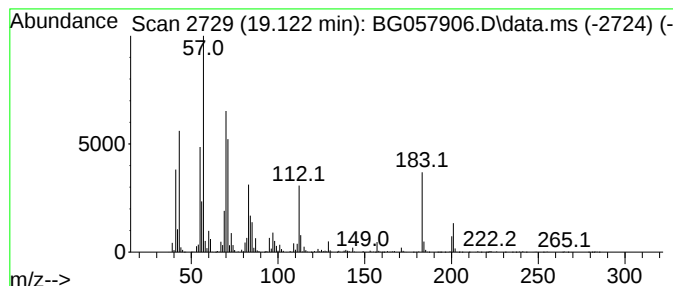
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Carbonic acid, 2-ethylhexyl... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.122	129.52 ng	5791120	Phenanthrene-d10	17.307

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, 2-ethylhexyl nonyl...	300	C18H36O3	1000383-13-6	72
2			Carbonic acid, 2-ethylhexyl unde...	328	C20H40O3	1000383-13-8	64
3			Dodecanoic acid, isooctyl ester	312	C20H40O2	084713-06-4	58
4			Dichloroacetic acid, 2-ethylhexy...	240	C10H18Cl2O2	068144-72-9	53
5			Decane, 5,6-dipropyl-	226	C16H34	119209-20-0	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
Data File : BG057906.D
Acq On : 29 Jun 2023 16:03
Operator : CG/JU
Sample : 03324-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

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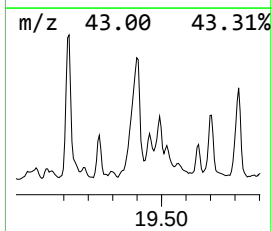
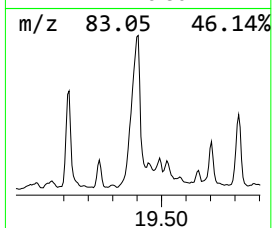
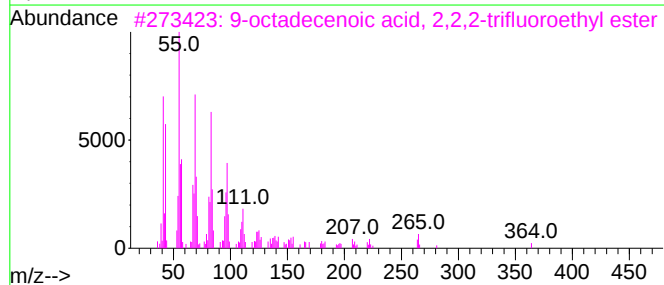
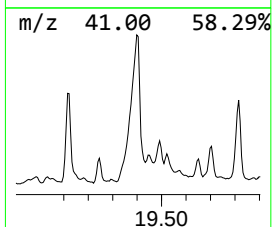
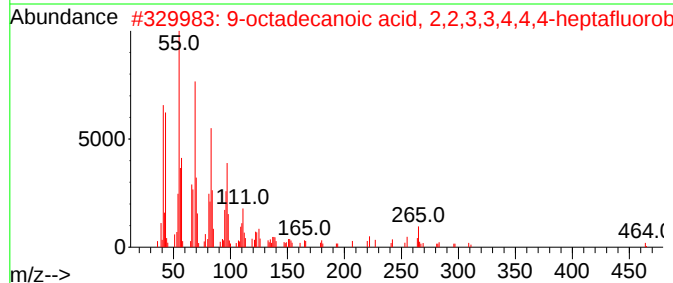
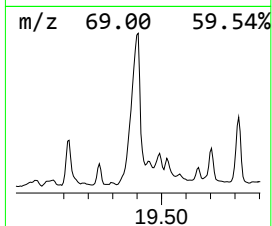
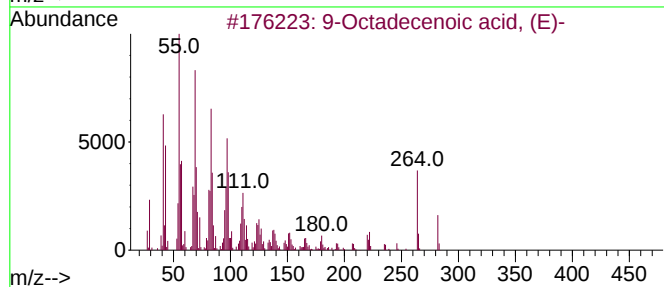
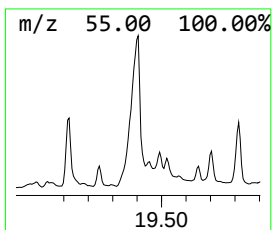
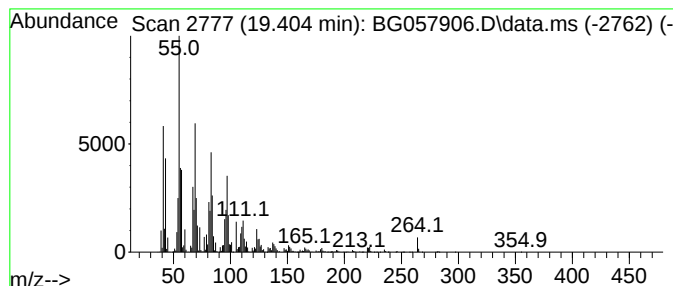
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 9-Octadecenoic acid, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.404	348.99 ng	15603900	Phenanthrene-d10	17.307

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	91
2			9-octadecanoic acid, 2,2,3,3,4,4...	464	C22H35F7O2	1000376-61-4	90
3			9-octadecenoic acid, 2,2,2-trifl...	364	C20H35F3O2	1000376-54-3	86
4			Cyclopentadecane	210	C15H30	000295-48-7	86
5			cis-Vaccenic acid	282	C18H34O2	000506-17-2	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
Data File : BG057906.D
Acq On : 29 Jun 2023 16:03
Operator : CG/JU
Sample : 03324-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EFF-WW

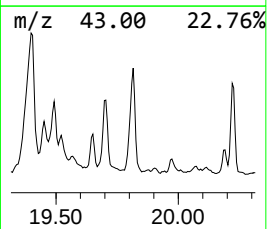
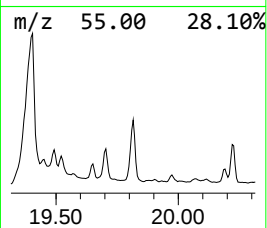
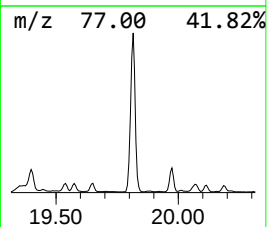
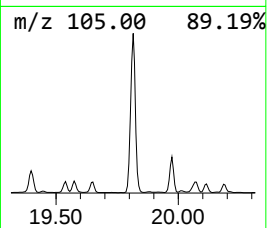
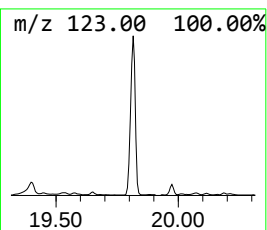
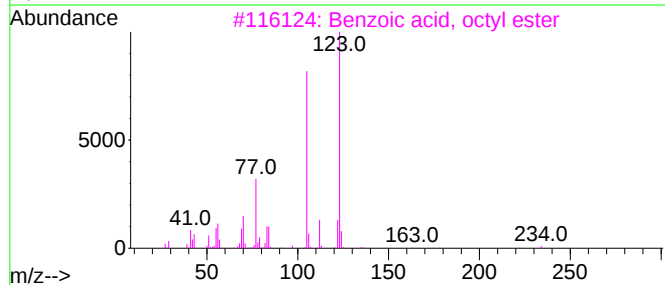
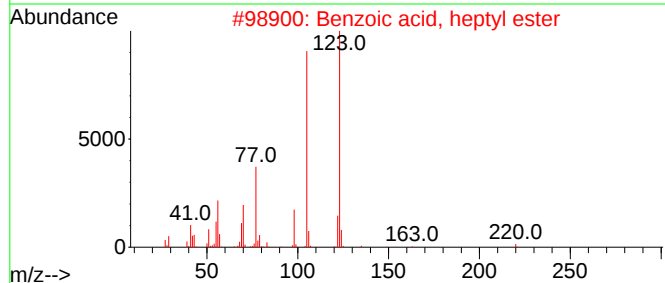
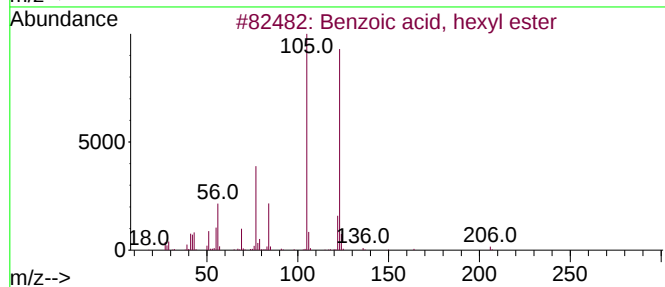
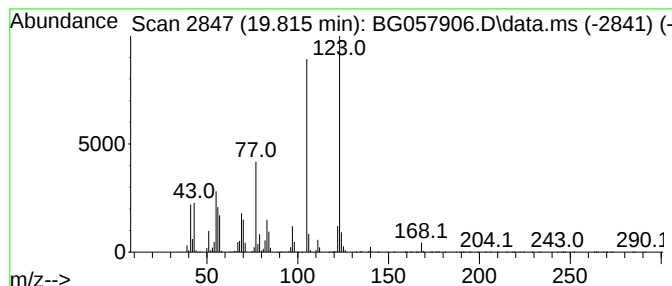
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Benzoic acid, hexyl ester Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.815	145.14 ng	6290180	Chrysene-d12	21.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, hexyl ester	206	C13H18O2	006789-88-4	80
2			Benzoic acid, heptyl ester	220	C14H20O2	007155-12-6	80
3			Benzoic acid, octyl ester	234	C15H22O2	000094-50-8	72
4			Benzoic acid, pentyl ester	192	C12H16O2	002049-96-9	53
5			Benzoic acid, octadecyl ester	374	C25H42O2	010578-34-4	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
Data File : BG057906.D
Acq On : 29 Jun 2023 16:03
Operator : CG/JU
Sample : 03324-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EFF-WW

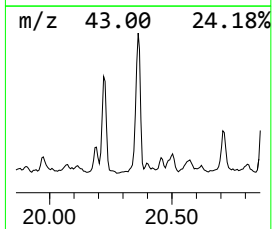
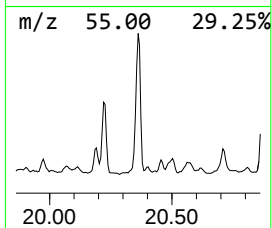
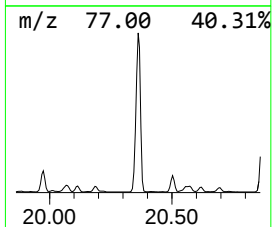
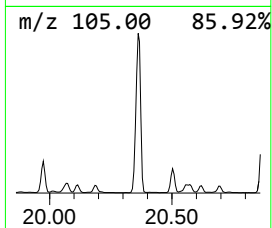
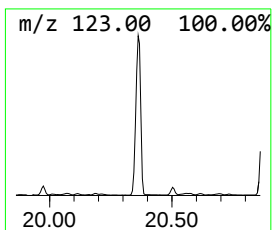
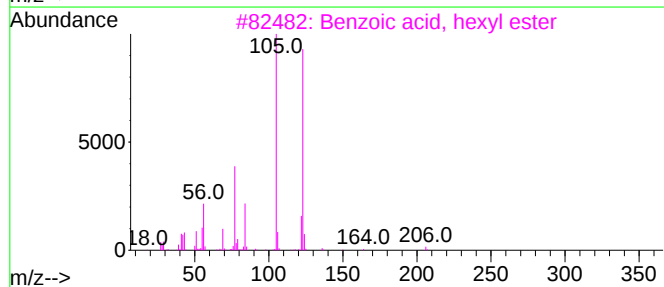
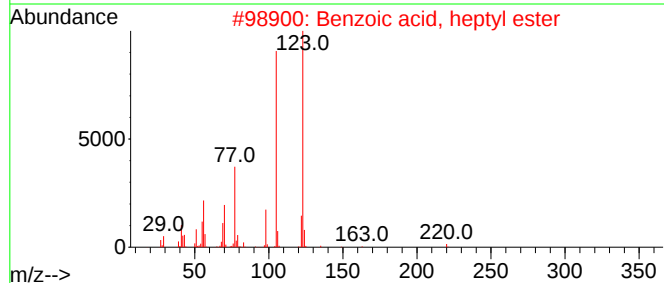
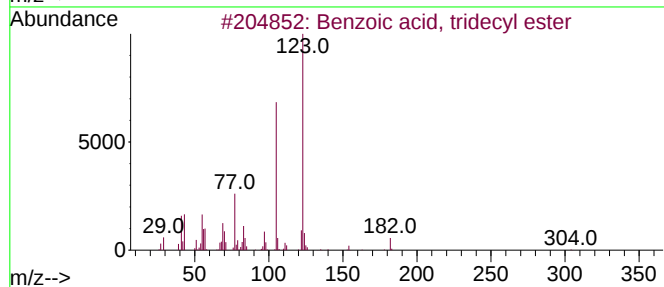
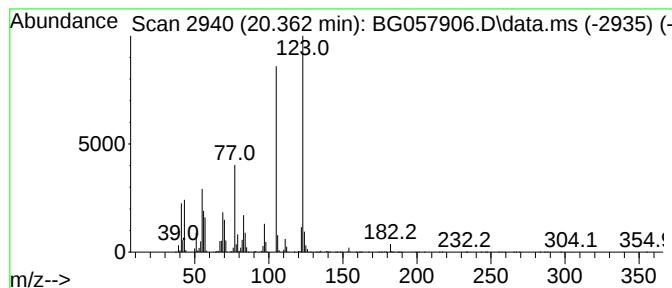
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Benzoic acid, tridecyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.362	159.76 ng	6923540	Chrysene-d12	21.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, tridecyl ester	304	C20H32O2	1010340-22-6	91
2			Benzoic acid, heptyl ester	220	C14H20O2	007155-12-6	86
3			Benzoic acid, hexyl ester	206	C13H18O2	006789-88-4	78
4			Benzoic acid, octyl ester	234	C15H22O2	000094-50-8	72
5			Benzoic acid, undecyl ester	276	C18H28O2	006316-30-9	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
Data File : BG057906.D
Acq On : 29 Jun 2023 16:03
Operator : CG/JU
Sample : 03324-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

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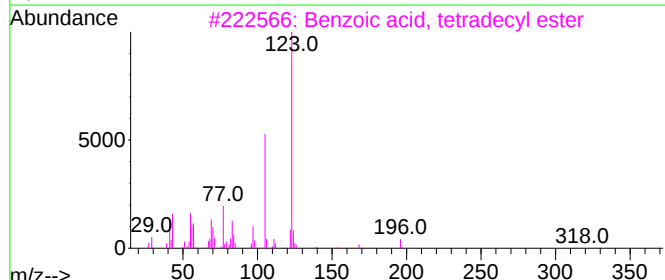
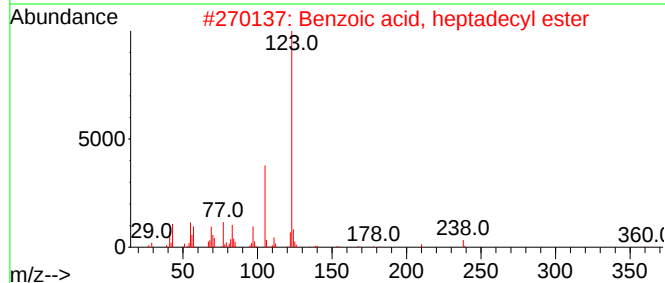
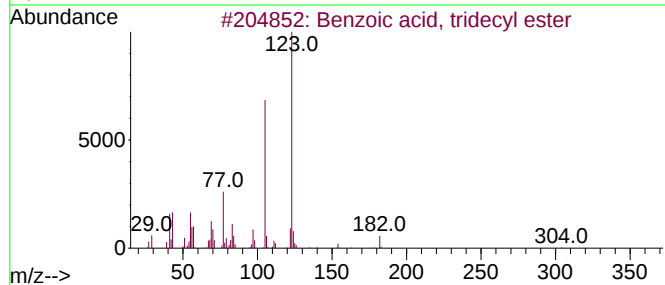
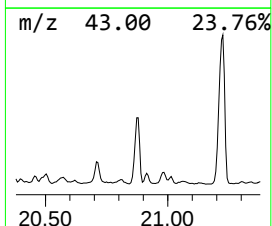
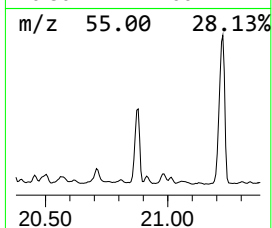
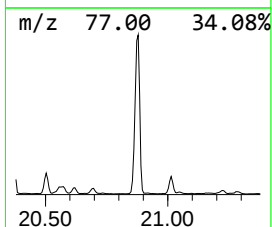
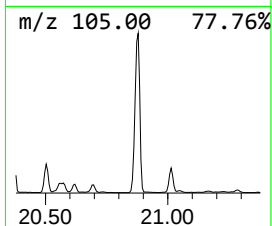
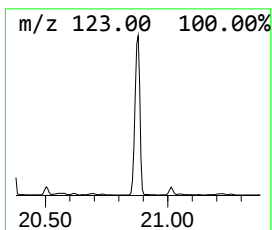
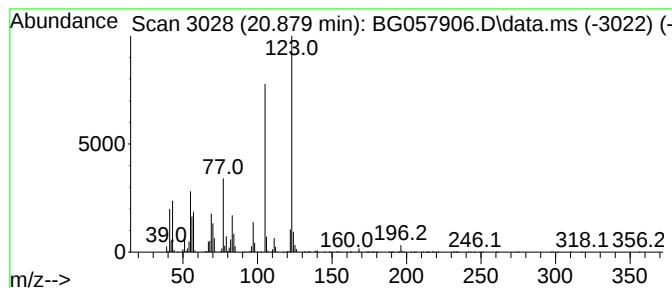
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Benzoic acid, heptadecyl ester Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.879	146.51 ng	6349670	Chrysene-d12	21.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, tridecyl ester	304	C20H32O2	1010340-22-6	91
2			Benzoic acid, heptadecyl ester	360	C24H40O2	1000340-23-0	86
3			Benzoic acid, tetradecyl ester	318	C21H34O2	1000340-22-7	83
4			Benzoic acid, nonadecyl ester	388	C26H44O2	1000340-23-2	80
5			Benzoic acid, undecyl ester	276	C18H28O2	006316-30-9	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
Data File : BG057906.D
Acq On : 29 Jun 2023 16:03
Operator : CG/JU
Sample : 03324-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

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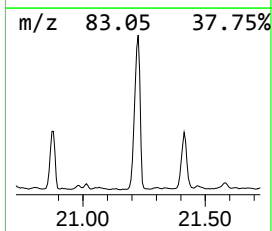
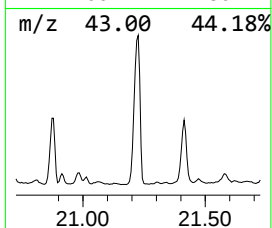
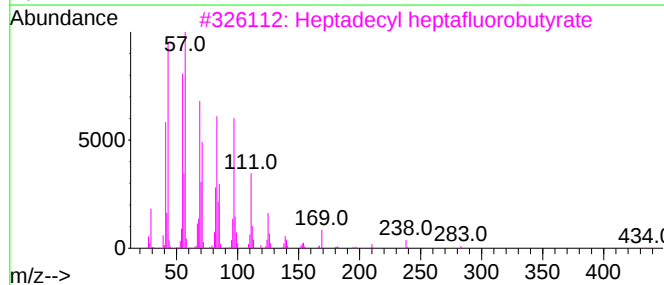
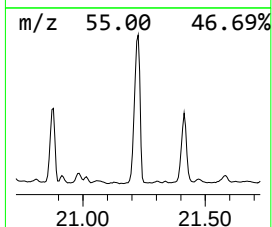
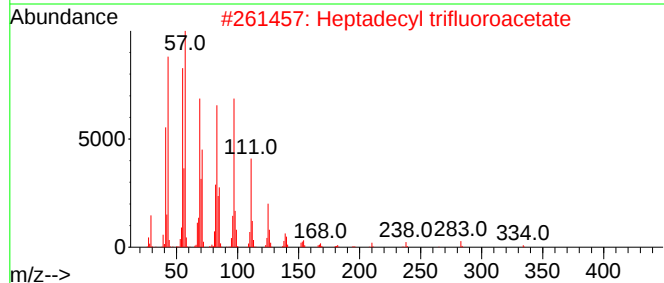
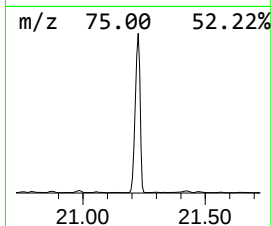
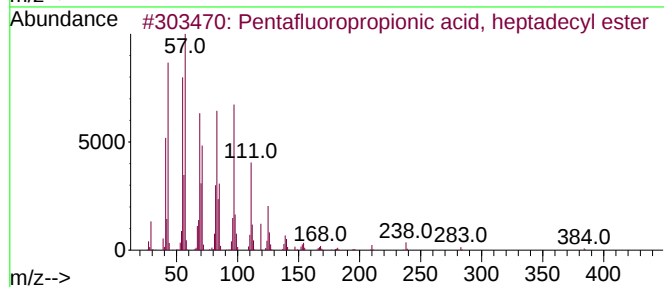
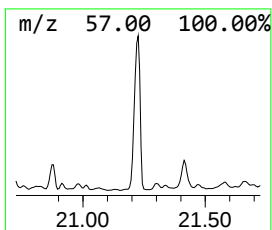
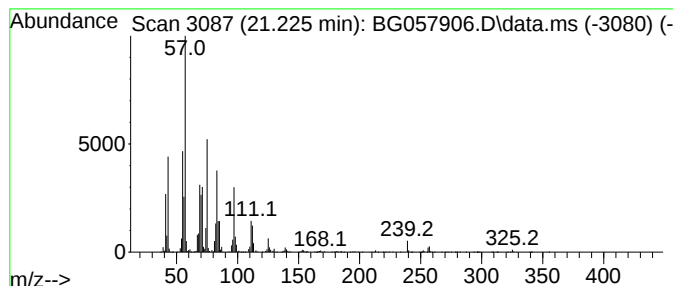
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Pentafluoropropionic acid, ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.225	264.39 ng	11458200	Chrysene-d12	21.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	60
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	60
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	60
4			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	53
5			Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
Data File : BG057906.D
Acq On : 29 Jun 2023 16:03
Operator : CG/JU
Sample : 03324-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

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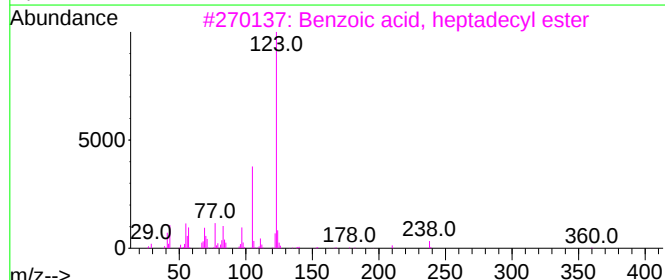
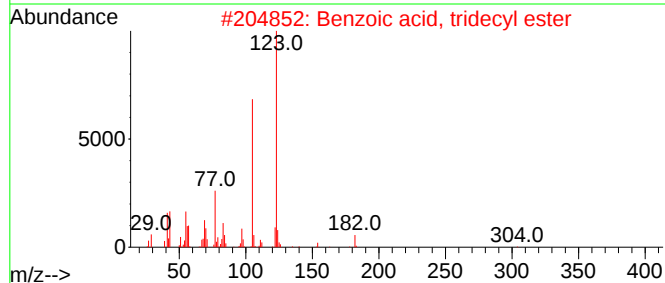
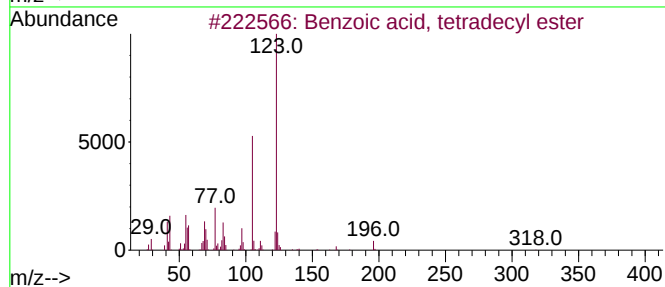
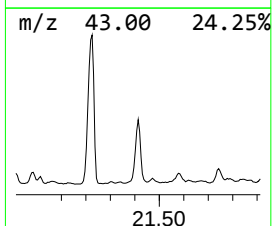
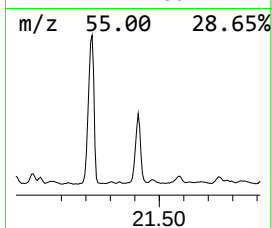
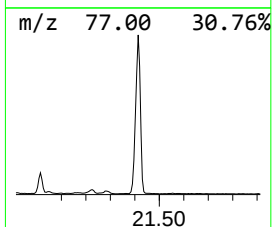
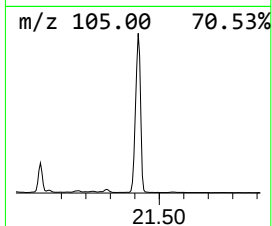
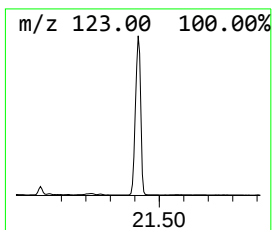
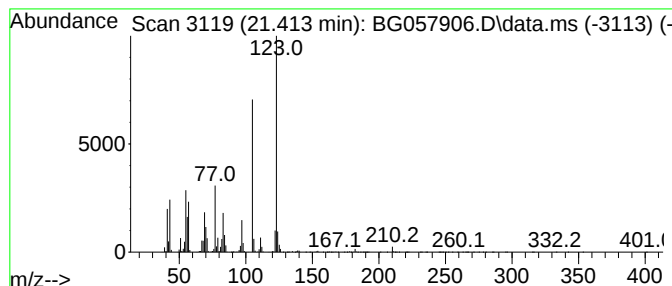
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Benzoic acid, tetradecyl ester Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.413	140.13 ng	6073100	Chrysene-d12	21.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, tetradecyl ester	318	C21H34O2	1000340-22-7	91
2			Benzoic acid, tridecyl ester	304	C20H32O2	1010340-22-6	91
3			Benzoic acid, heptadecyl ester	360	C24H40O2	1000340-23-0	90
4			Benzoic acid, octadecyl ester	374	C25H42O2	010578-34-4	86
5			Eicosyl benzoate	402	C27H46O2	103098-99-3	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
Data File : BG057906.D
Acq On : 29 Jun 2023 16:03
Operator : CG/JU
Sample : 03324-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EFF-WW

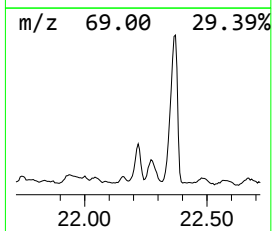
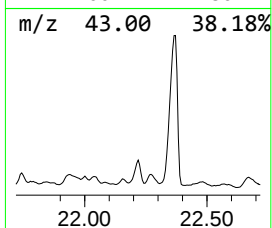
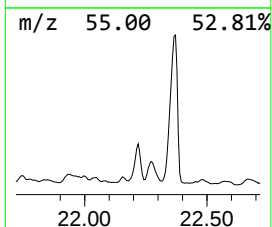
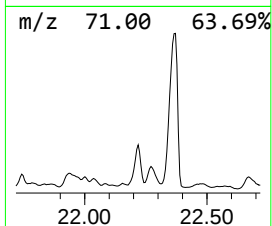
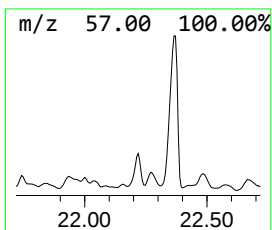
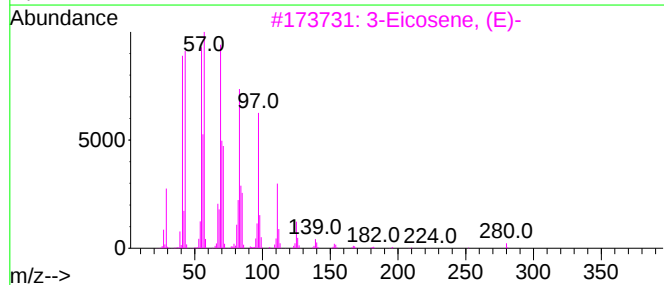
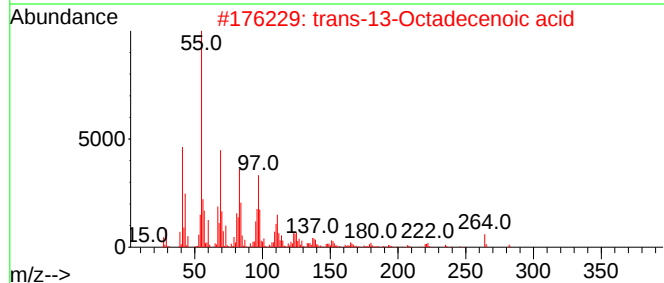
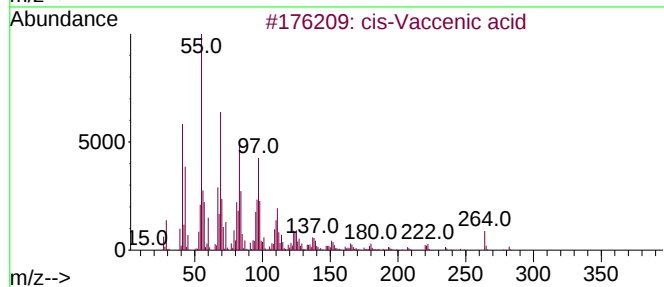
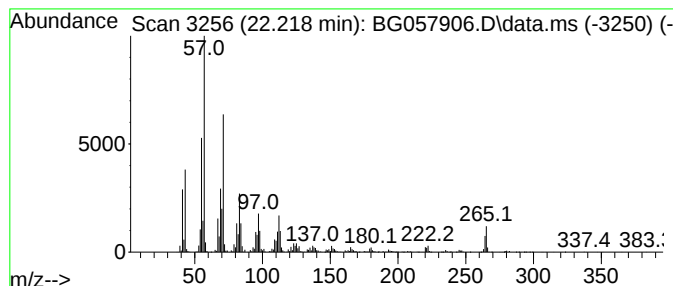
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 cis-Vaccenic acid Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.218	68.22 ng	2956440	Chrysene-d12	21.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-Vaccenic acid	282	C18H34O2	000506-17-2	83
2			trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	80
3			3-Eicosene, (E)-	280	C20H40	074685-33-9	51
4			9-Eicosene, (E)-	280	C20H40	074685-29-3	51
5			Decane, 1,1'-oxybis-	298	C20H42O	002456-28-2	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
Data File : BG057906.D
Acq On : 29 Jun 2023 16:03
Operator : CG/JU
Sample : 03324-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EFF-WW

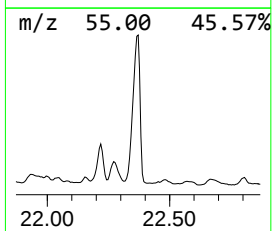
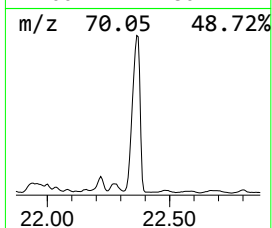
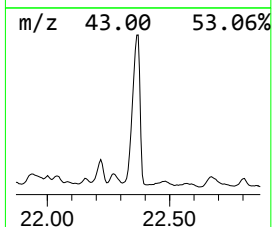
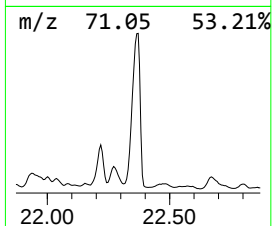
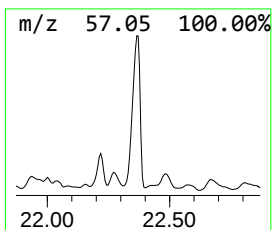
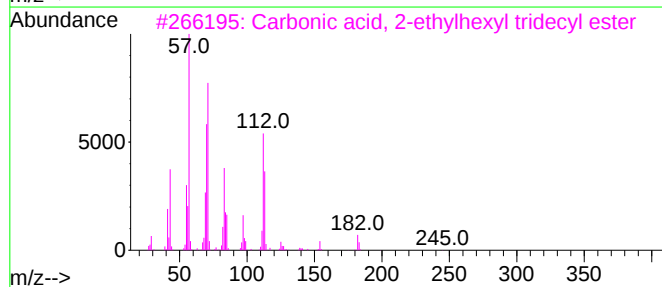
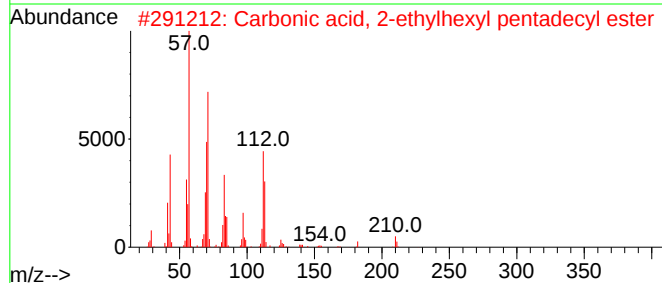
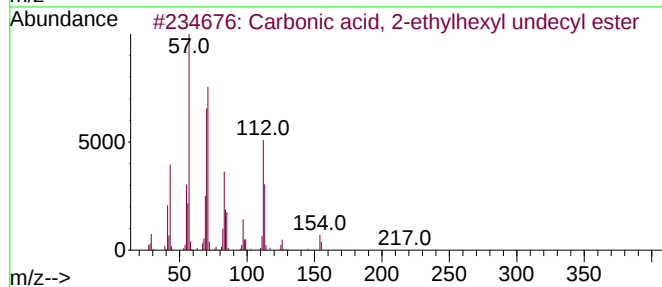
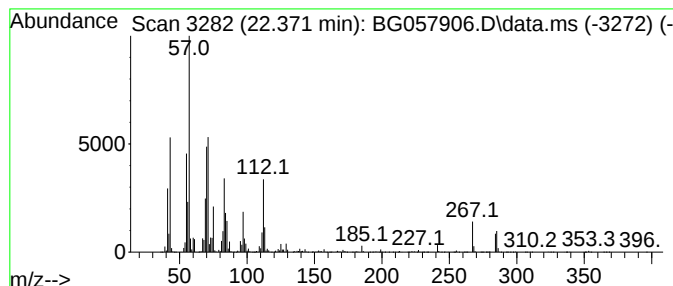
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Carbonic acid, 2-ethylhexyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.371	381.48 ng	16532600	Chrysene-d12	21.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, 2-ethylhexyl unde...	328	C20H40O3	1000383-13-8	64
2			Carbonic acid, 2-ethylhexyl pent...	384	C24H48O3	1000383-14-2	64
3			Carbonic acid, 2-ethylhexyl trid...	356	C22H44O3	1000383-14-0	64
4			Carbonic acid, 2-ethylhexyl nony...	300	C18H36O3	1000383-13-6	53
5			Isobutyl octan-2-yl carbonate	230	C13H26O3	1000372-74-7	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
Data File : BG057906.D
Acq On : 29 Jun 2023 16:03
Operator : CG/JU
Sample : 03324-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EFF-WW

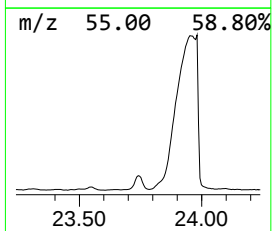
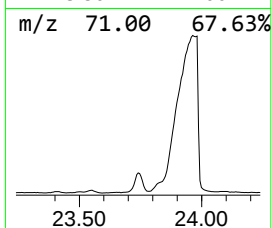
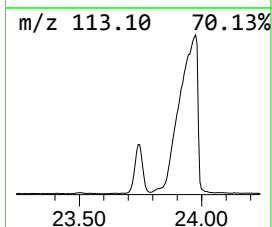
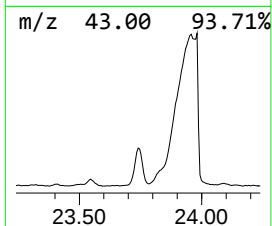
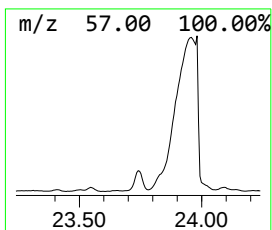
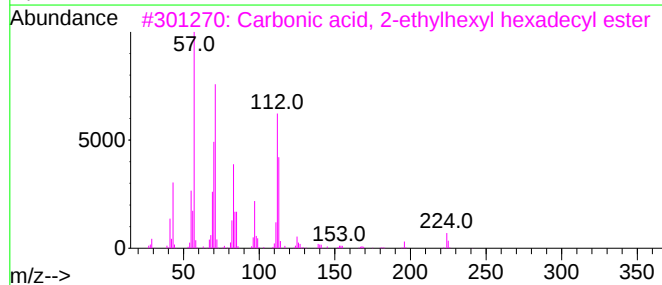
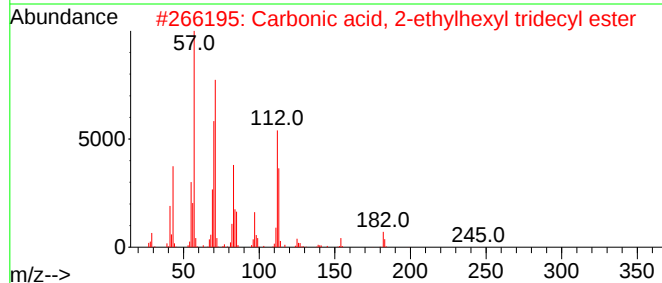
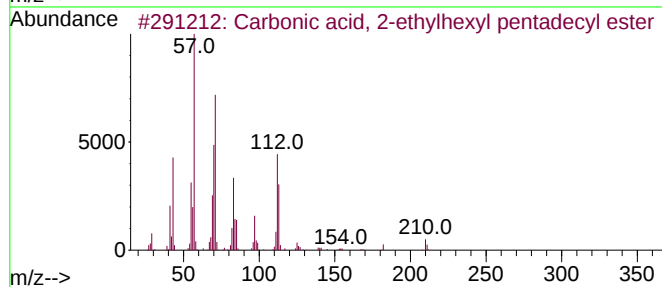
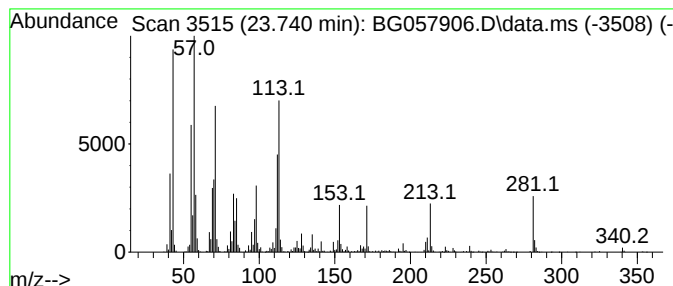
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown23.740 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.740	65.60 ng	3003960	Perylene-d12	24.709

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, 2-ethylhexyl pent...	384	C24H48O3	1000383-14-2	41
2			Carbonic acid, 2-ethylhexyl trid...	356	C22H44O3	1000383-14-0	41
3			Carbonic acid, 2-ethylhexyl hexa...	398	C25H50O3	1000383-14-3	41
4			Carbonic acid, 2-ethylhexyl hept...	412	C26H52O3	1000383-14-4	38
5			CITRONELLAL, DIHYDRO-	156	C10H20O	005988-91-0	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
Data File : BG057906.D
Acq On : 29 Jun 2023 16:03
Operator : CG/JU
Sample : 03324-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

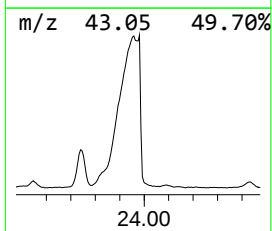
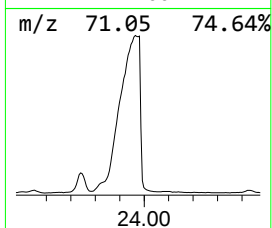
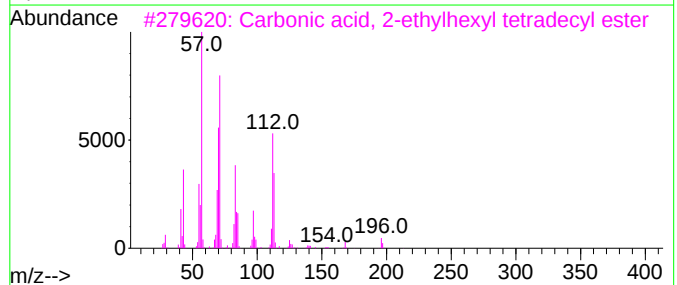
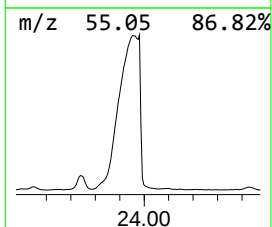
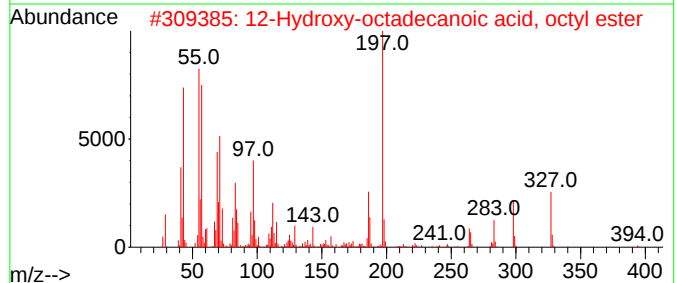
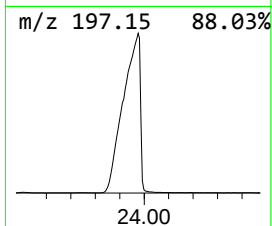
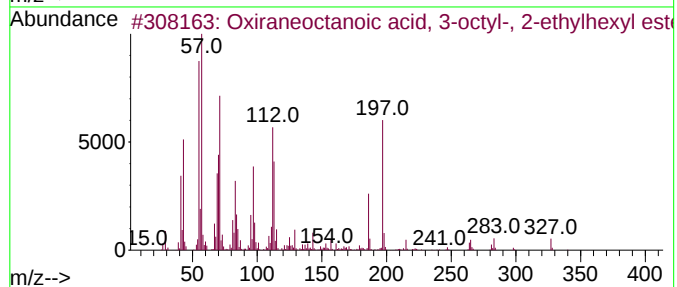
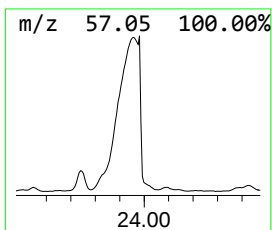
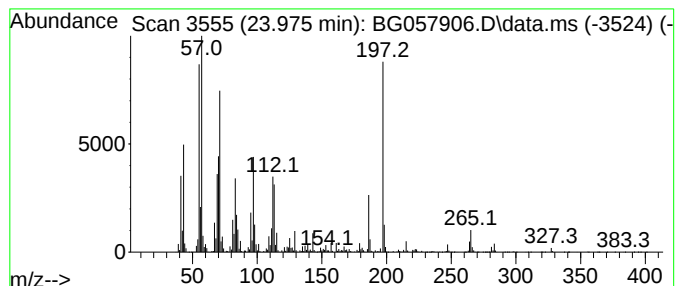
Instrument :
BNA_G
ClientSampleId :
EFF-WW

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Oxiraneoctanoic acid, 3-oct... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
23.975	1288.55 ng	59005900	Perylene-d12		24.709	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Oxiraneoctanoic acid, 3-octyl-, ...		410	C26H50O3	000141-38-8	83
2	12-Hydroxy-octadecanoic acid, oc...		412	C26H52O3	074819-90-2	58
3	Carbonic acid, 2-ethylhexyl tetr...		370	C23H46O3	1010383-14-1	43
4	Carbonic acid, 2-ethylhexyl pent...		384	C24H48O3	1000383-14-2	43
5	Decane, 5,6-dipropyl-		226	C16H34	119209-20-0	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
 Data File : BG057906.D
 Acq On : 29 Jun 2023 16:03
 Operator : CG/JU
 Sample : 03324-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 EFF-WW

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.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-Hexanol, 2-et...	8.100	1881.2	ng	66043500	1	7.917	702136	20.0
n-Decanoic acid	13.082	414.2	ng	24270700	3	14.551	1172040	20.0
Undecanoic acid	15.197	911.4	ng	53409600	3	14.551	1172040	20.0
Hexanoic acid, ...	15.890	103.3	ng	6053080	3	14.551	1172040	20.0
1-Octanol, 5,7,...	16.478	77.8	ng	3479900	4	17.307	894243	20.0
3-Eicosene, (E)-	16.531	154.2	ng	6893630	4	17.307	894243	20.0
3-Chloropropion...	16.578	107.0	ng	4783500	4	17.307	894243	20.0
Tetradecanoic acid	16.872	1023.6	ng	45767500	4	17.307	894243	20.0
n-Hexadecanoic ...	18.288	645.3	ng	28851400	4	17.307	894243	20.0
Carbonic acid, ...	19.122	129.5	ng	5791120	4	17.307	894243	20.0
9-Octadecenoic ...	19.404	349.0	ng	15603900	4	17.307	894243	20.0
Benzoic acid, h...	19.815	145.1	ng	6290180	5	21.554	866767	20.0
Benzoic acid, t...	20.362	159.8	ng	6923540	5	21.554	866767	20.0
Benzoic acid, h...	20.879	146.5	ng	6349670	5	21.554	866767	20.0
Pentafluoroprop...	21.225	264.4	ng	11458200	5	21.554	866767	20.0
Benzoic acid, t...	21.413	140.1	ng	6073100	5	21.554	866767	20.0
cis-Vaccenic acid	22.218	68.2	ng	2956440	5	21.554	866767	20.0
Carbonic acid, ...	22.371	381.5	ng	16532600	5	21.554	866767	20.0
unknown23.740	23.740	65.6	ng	3003960	6	24.709	915850	20.0
Oxiraneoctanoic...	23.975	1288.6	ng	59005900	6	24.709	915850	20.0