

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
 Data File : BG057907.D
 Acq On : 29 Jun 2023 16:44
 Operator : CG/JU
 Sample : 03375-02
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-5(8-10)

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: BG057907.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.020	324	329	338	rVB	39997	58795	1.65%	0.359%
2	5.490	402	409	428	rVB	710402	1180213	33.21%	7.200%
3	7.082	673	680	701	rBV	711243	1257869	35.40%	7.674%
4	7.916	815	822	829	rBV	171721	286128	8.05%	1.746%
5	9.074	1011	1019	1028	rBV	409574	722881	20.34%	4.410%
6	10.719	1290	1299	1307	rVB	227791	402152	11.32%	2.453%
7	13.175	1710	1717	1725	rVB	988308	1502838	42.29%	9.169%
8	14.550	1945	1951	1960	rBV	355588	552368	15.54%	3.370%
9	15.907	2176	2182	2188	rBV	75181	105856	2.98%	0.646%
10	16.036	2198	2204	2218	rBV	844190	1342761	37.79%	8.192%
11	17.294	2412	2418	2425	rBV	484150	710561	20.00%	4.335%
12	19.914	2858	2864	2873	rBV	1764251	2363604	66.51%	14.420%
13	20.707	2997	2999	3003	rVB	41514	41422	1.17%	0.253%
14	21.201	3079	3083	3090	rVB3	260770	412095	11.60%	2.514%
15	21.371	3099	3112	3135	rVB2	707070	3553524	100.00%	21.679%
16	21.547	3137	3142	3153	rVB2	472081	779273	21.93%	4.754%
17	21.741	3171	3175	3180	rBV	95761	134668	3.79%	0.822%
18	22.335	3272	3276	3285	rVB	89105	155078	4.36%	0.946%
19	24.697	3671	3678	3688	rVB	300454	829231	23.34%	5.059%

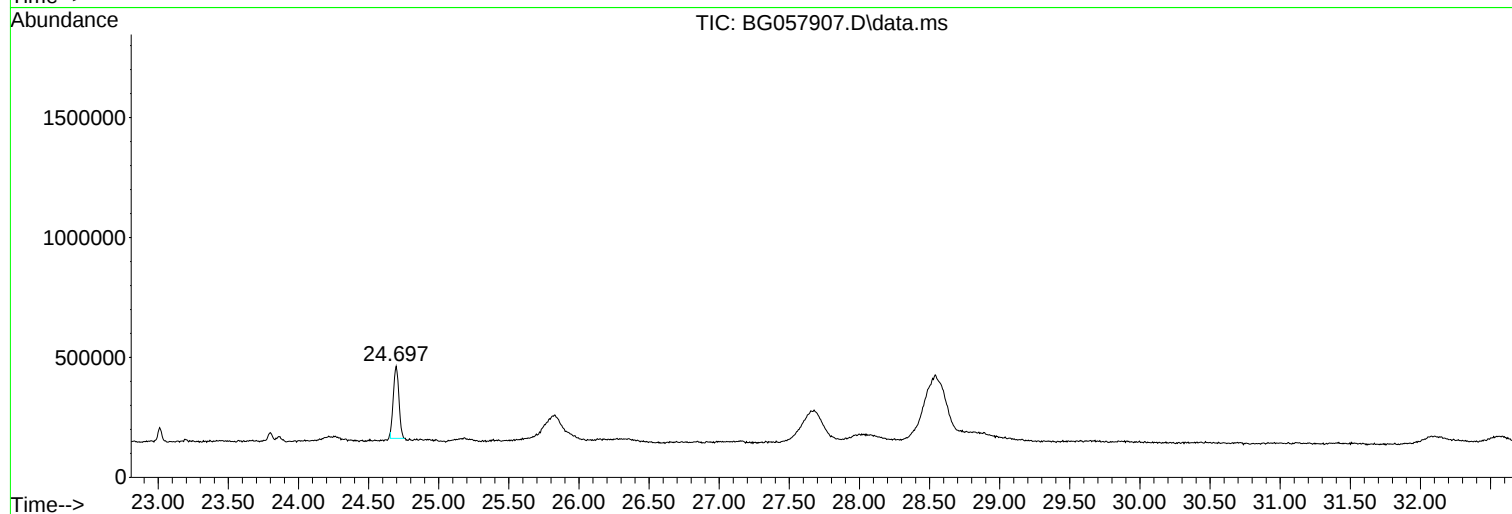
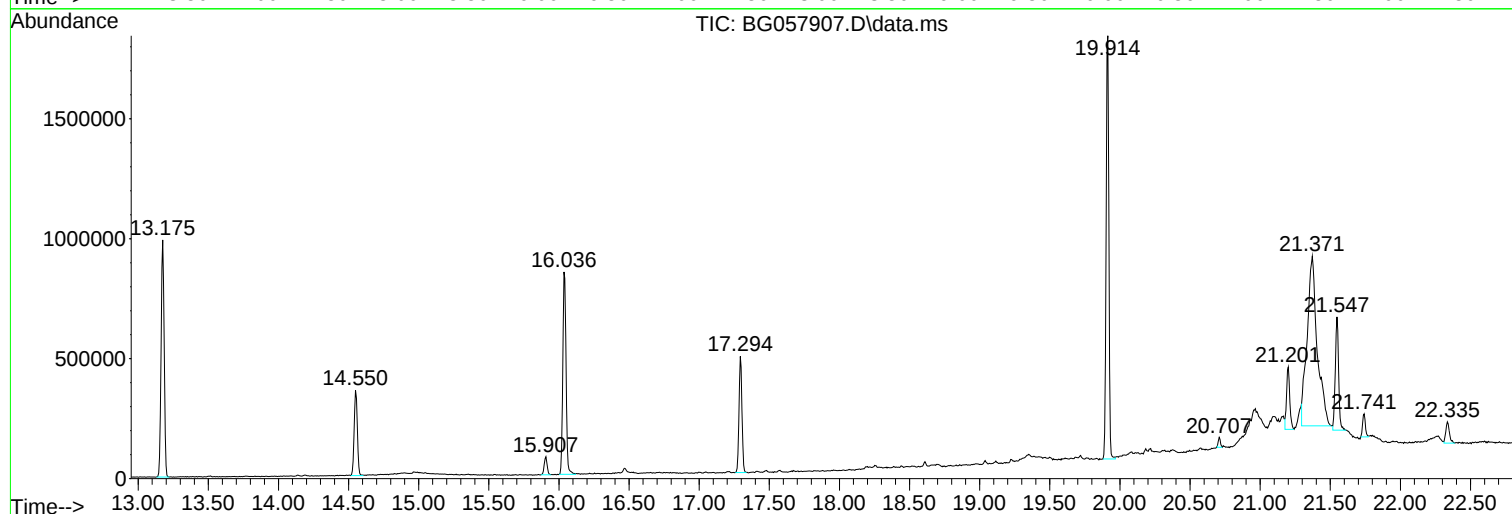
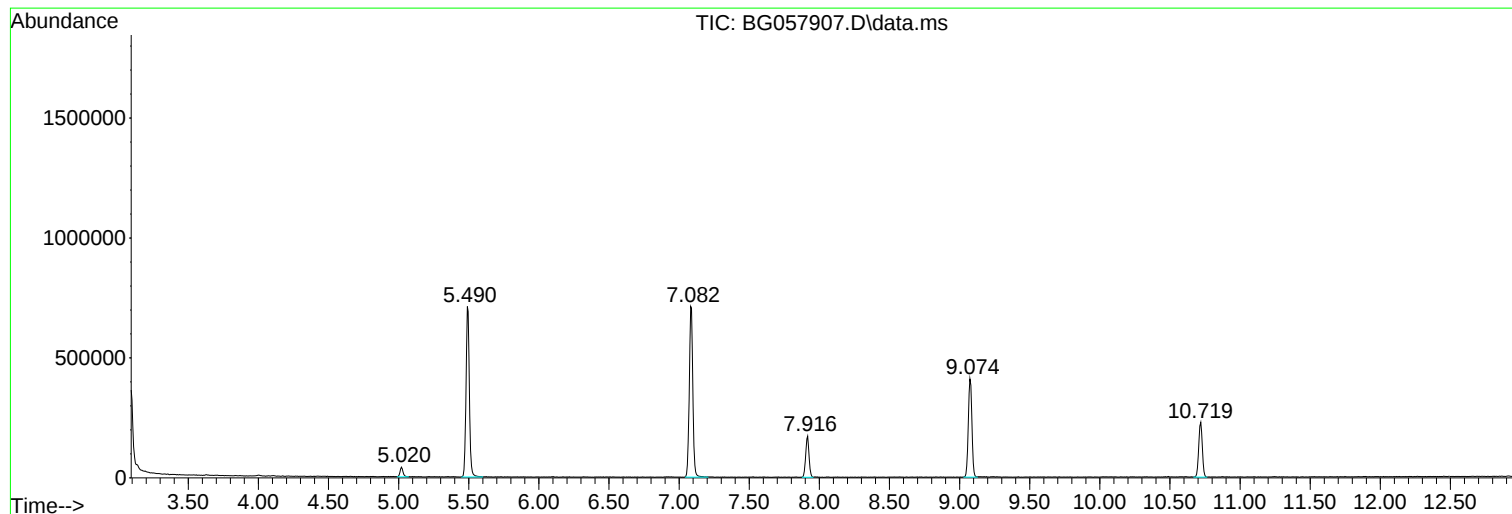
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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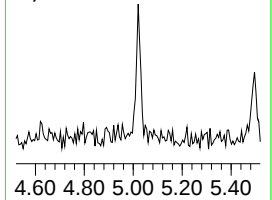
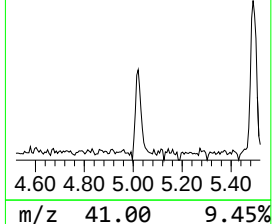
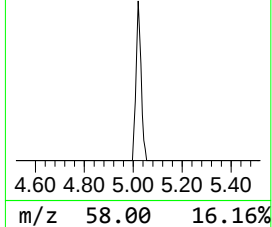
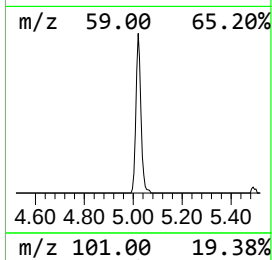
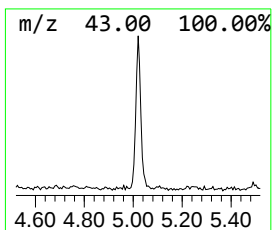
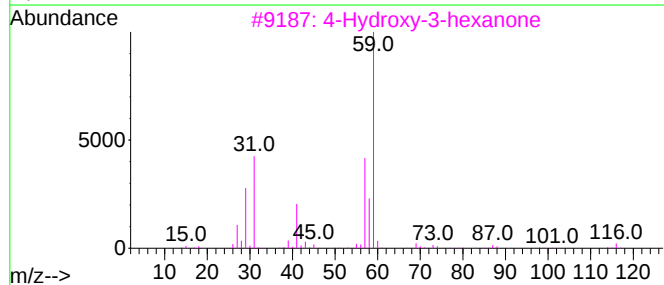
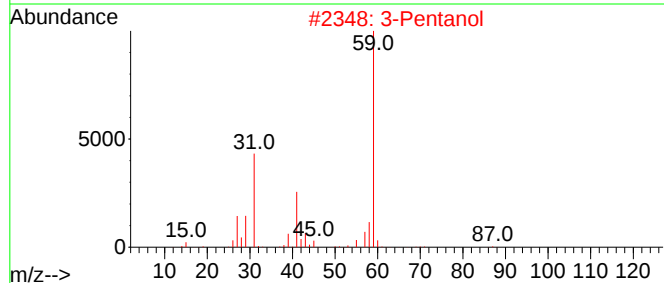
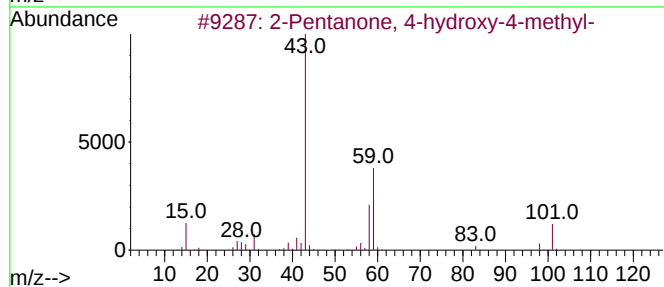
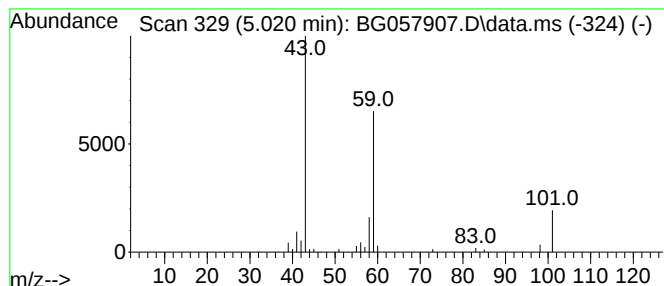
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.020	4.11 ng	58795	1,4-Dichlorobenzene-d4	7.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	3-Pentanol	88	C5H12O	000584-02-1	25		
3	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	23		
4	4-Pentene-2-ol, 2-methyl	100	C6H12O	000624-97-5	17		
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9		



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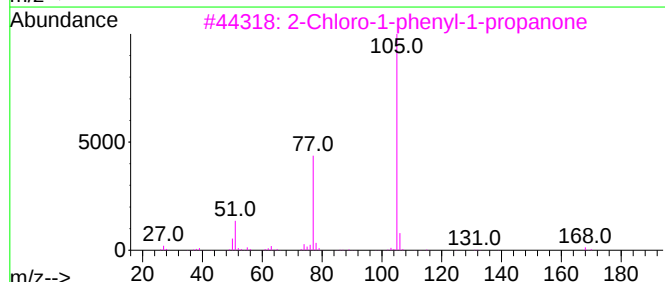
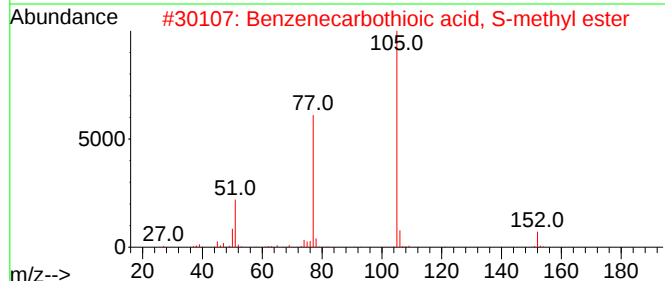
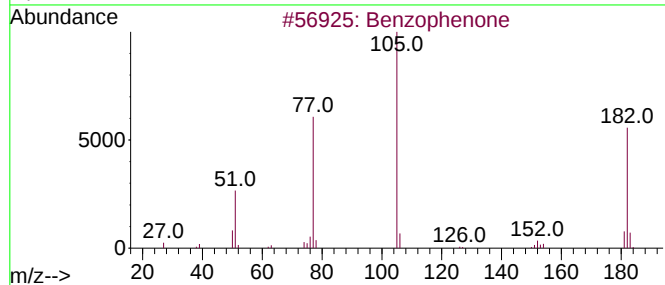
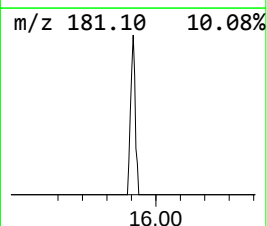
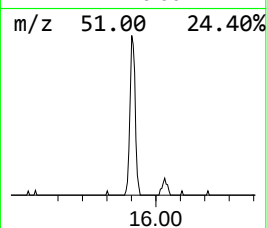
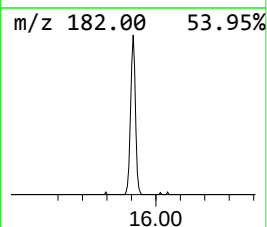
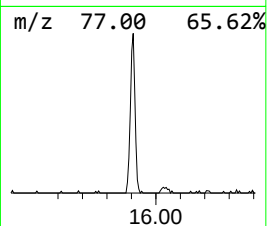
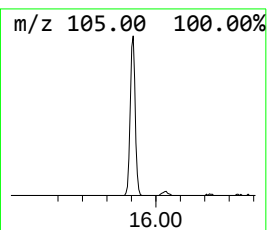
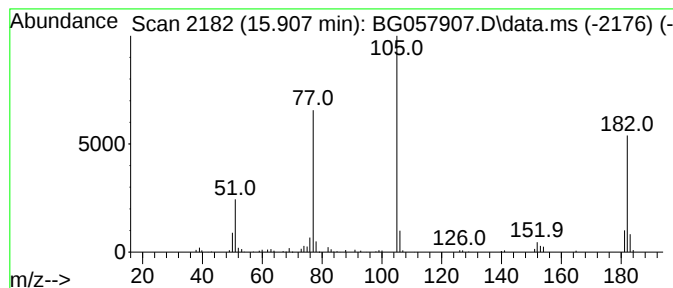
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Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.907	3.83 ng	105856	Acenaphthene-d10	14.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
3			2-Chloro-1-phenyl-1-propanone	168	C9H9ClO	006084-17-9	47
4			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47
5			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47



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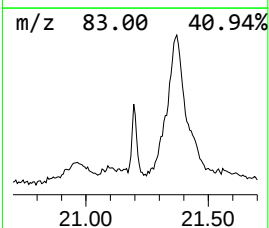
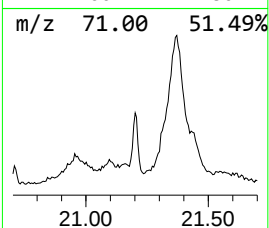
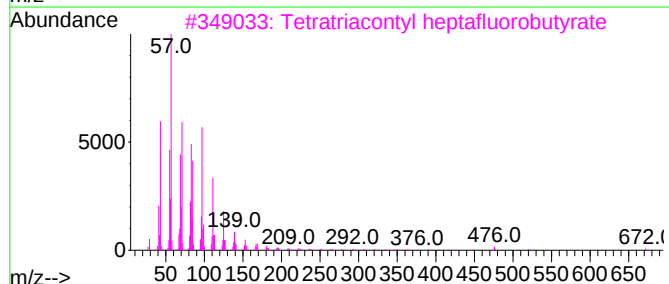
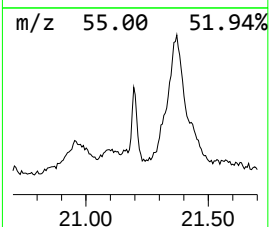
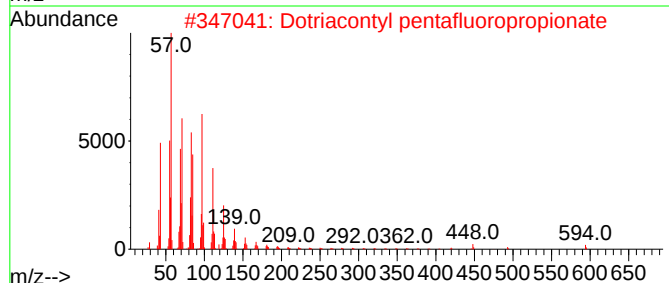
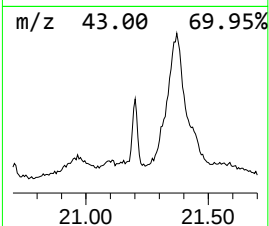
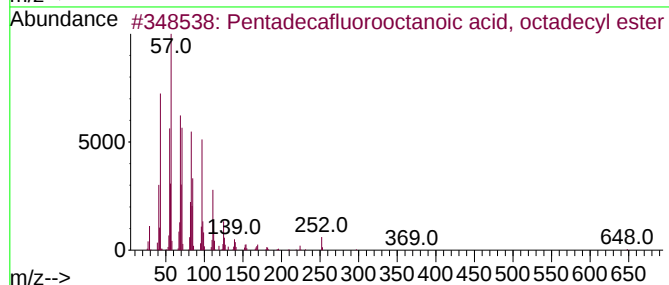
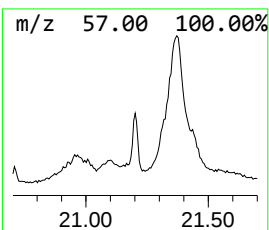
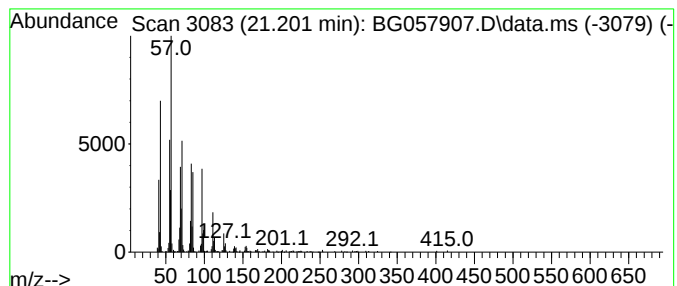
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Peak Number 3 Pentadecafluorooctanoic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.201	10.58 ng	412095	Chrysene-d12	21.547

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
2			Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1010351-81-4	91
3			Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	91
4			1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
5			Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91



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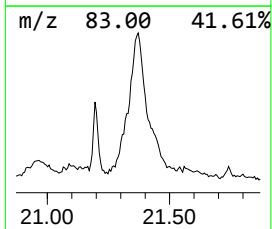
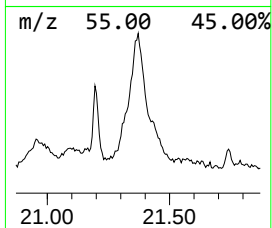
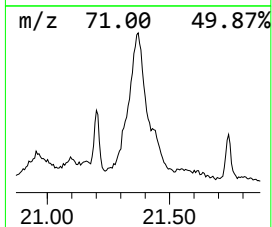
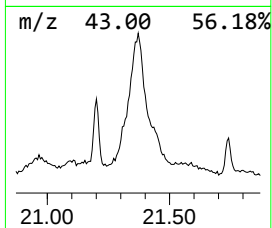
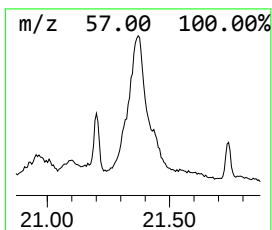
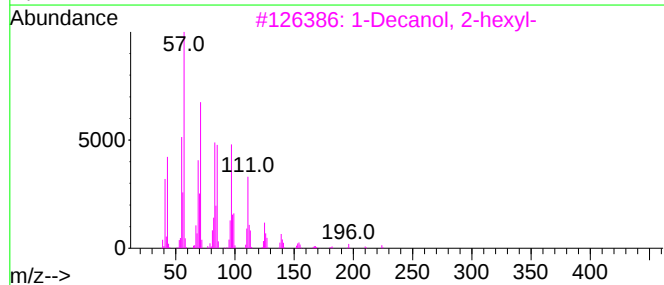
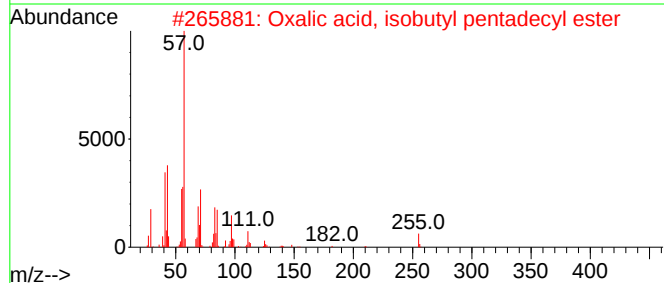
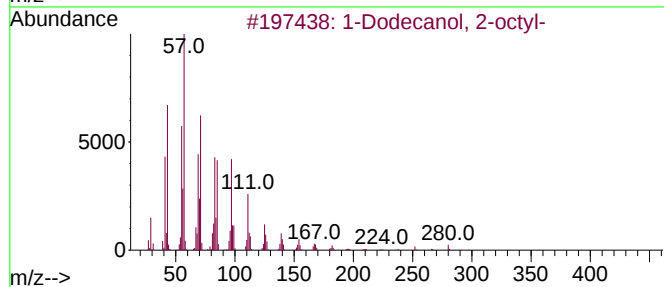
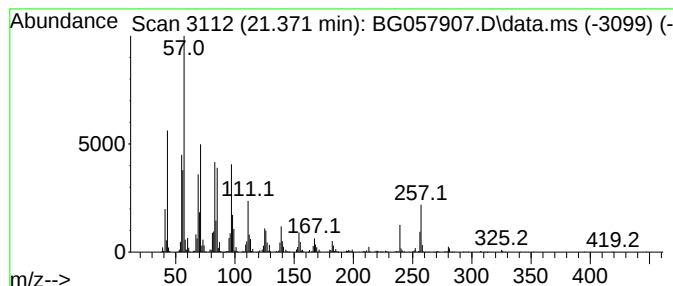
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Peak Number 4 1-Dodecanol, 2-octyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.371	91.20 ng	3553520	Chrysene-d12	21.547

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-			298	C20H42O	005333-42-6	93
2	Oxalic acid, isobutyl pentadecyl...			356	C21H40O4	1000309-38-0	76
3	1-Decanol, 2-hexyl-			242	C16H34O	002425-77-6	72
4	1-Decanol, 2-octyl-			270	C18H38O	045235-48-1	70
5	Oxalic acid, isobutyl octadecyl ...			398	C24H46O4	1000309-38-3	68



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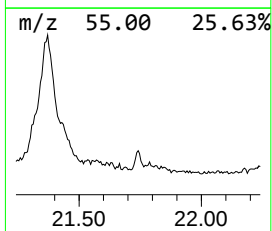
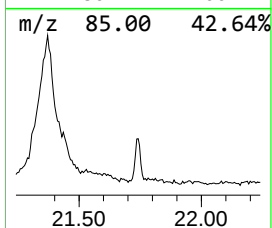
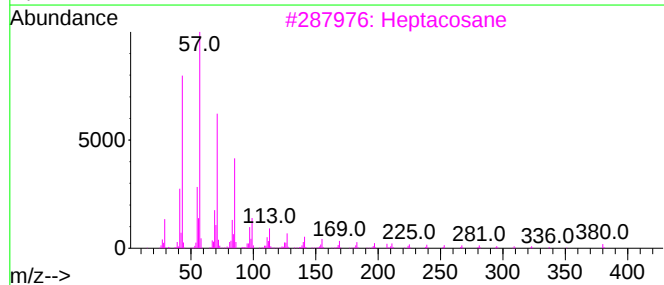
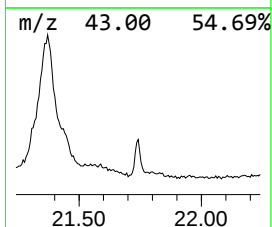
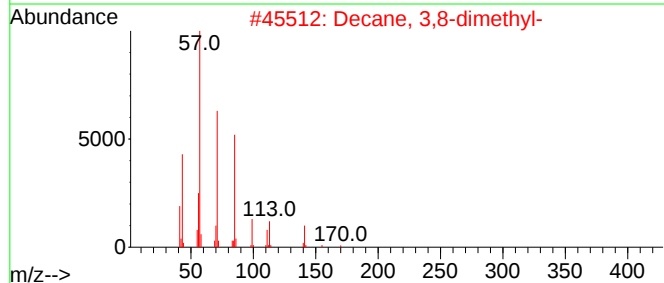
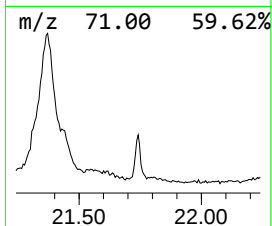
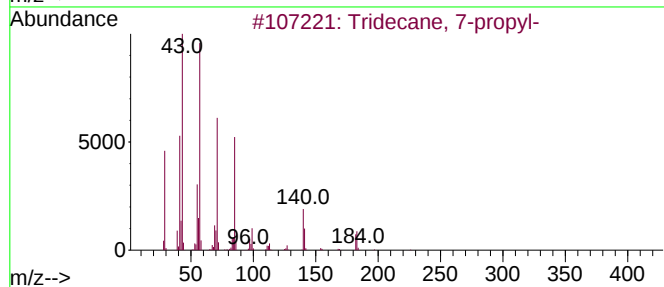
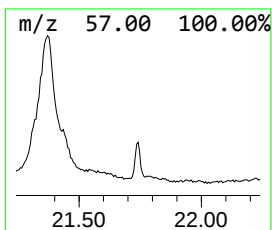
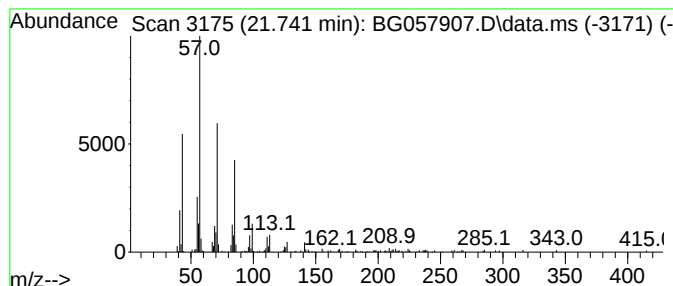
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Peak Number 5 Tridecane, 7-propyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.741	3.46 ng	134668	Chrysene-d12	21.547

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 7-propyl-	226	C16H34	055045-09-5	91
2			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	90
3			Heptacosane	380	C27H56	000593-49-7	90
4			Tetracosane	338	C24H50	000646-31-1	87
5			Hexacosane	366	C26H54	000630-01-3	86



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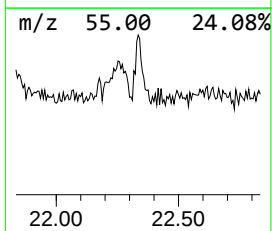
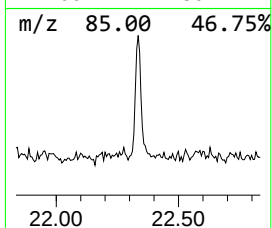
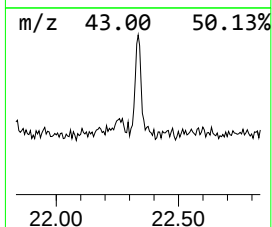
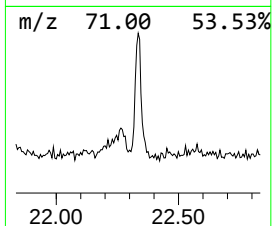
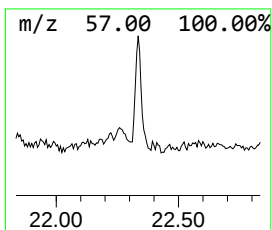
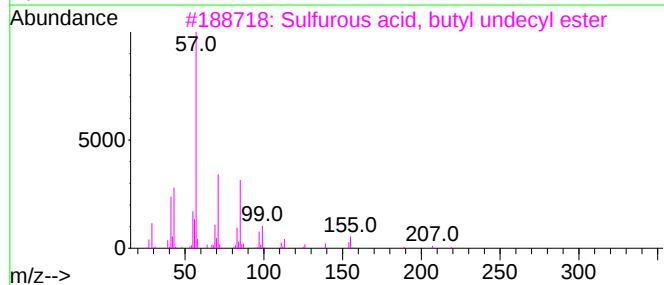
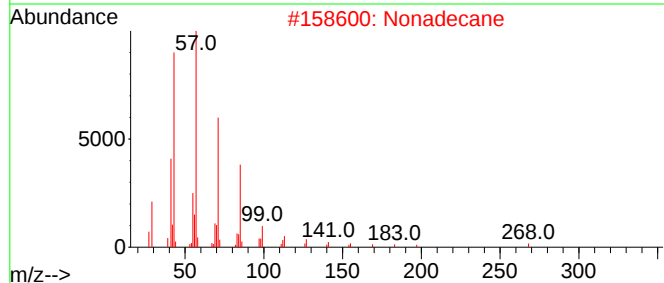
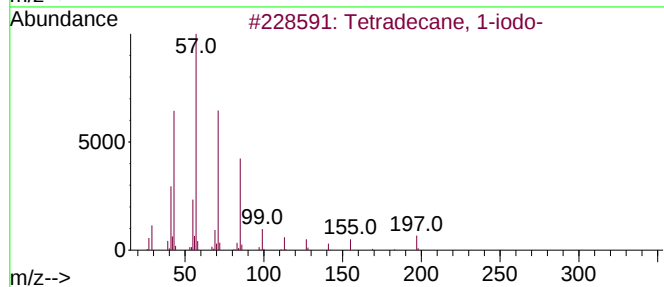
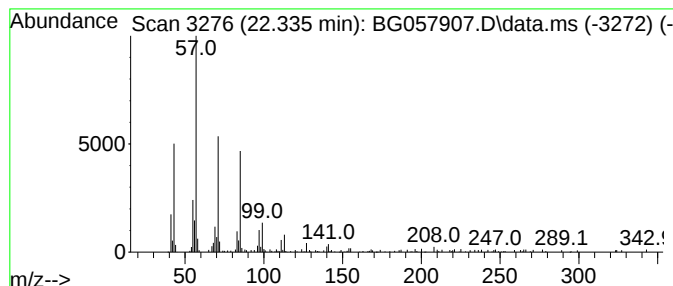
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tetradecane, 1-iodo- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.335	3.98 ng	155078	Chrysene-d12	21.547

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
2			Nonadecane	268	C19H40	000629-92-5	72
3			Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	64
4			Heptadecane	240	C17H36	000629-78-7	64
5			Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
Data File : BG057907.D
Acq On : 29 Jun 2023 16:44
Operator : CG/JU
Sample : 03375-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-5(8-10)

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.020	4.1	ng	58795	1	7.916	286128	20.0
Benzophenone	15.907	3.8	ng	105856	3	14.550	552368	20.0
Pentadecafluoro...	21.201	10.6	ng	412095	5	21.547	779273	20.0
1-Dodecanol, 2-...	21.371	91.2	ng	3553520	5	21.547	779273	20.0
Tridecane, 7-pr...	21.741	3.5	ng	134668	5	21.547	779273	20.0
Tetradecane, 1-...	22.335	4.0	ng	155078	5	21.547	779273	20.0