

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112021\
 Data File : BG051156.D
 Acq On : 20 Nov 2021 20:39
 Operator : CG/JU
 Sample : M4758-31
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP16

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-BG111921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG051156.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.263	297	302	311	rVB2	24332	37687	2.49%	0.487%
2	5.739	377	383	395	rVB	367053	618828	40.85%	7.995%
3	7.355	651	658	673	rBV	372405	686113	45.29%	8.864%
4	8.201	796	802	813	rVB	91185	156150	10.31%	2.017%
5	9.376	993	1002	1016	rBV	234991	438927	28.98%	5.671%
6	10.780	1236	1241	1250	rBV2	8063	16361	1.08%	0.211%
7	11.033	1276	1284	1296	rBV	118028	220446	14.55%	2.848%
8	13.454	1686	1696	1703	rBV	578928	892146	58.90%	11.526%
9	14.446	1859	1865	1874	rBV5	8387	16114	1.06%	0.208%
10	14.834	1922	1931	1939	rBV	196402	306798	20.25%	3.964%
11	16.186	2154	2161	2168	rVB5	13811	24497	1.62%	0.316%
12	16.321	2178	2184	2200	rBV	438332	685427	45.25%	8.856%
13	17.449	2371	2376	2382	rBV	15425	20467	1.35%	0.264%
14	17.584	2392	2399	2405	rBV	252038	397733	26.26%	5.139%
15	18.207	2500	2505	2513	rVB2	16193	22300	1.47%	0.288%
16	18.436	2540	2544	2553	rBV4	9469	15164	1.00%	0.196%
17	19.370	2700	2703	2707	rVB2	28279	30026	1.98%	0.388%
18	19.817	2775	2779	2784	rBV4	9886	15404	1.02%	0.199%
19	20.175	2834	2840	2845	rBV	1122585	1514805	100.00%	19.571%
20	20.945	2967	2971	2975	rVB2	16709	18760	1.24%	0.242%
21	21.468	3050	3060	3073	rBV2	87896	244686	16.15%	3.161%
22	21.573	3073	3078	3085	rVB	49964	79178	5.23%	1.023%
23	21.885	3124	3131	3142	rBV	265465	460459	30.40%	5.949%
24	22.032	3152	3156	3164	rBV2	18988	29237	1.93%	0.378%
25	22.666	3260	3264	3267	rBV2	18747	31407	2.07%	0.406%
26	22.696	3267	3269	3280	rVB9	18791	44743	2.95%	0.578%
27	23.395	3382	3388	3394	rVB2	19941	38298	2.53%	0.495%
28	24.235	3523	3531	3537	rBV3	26046	57215	3.78%	0.739%
29	25.281	3695	3709	3719	rVB2	149452	487942	32.21%	6.304%
30	26.421	3897	3903	3913	rVB3	24538	71585	4.73%	0.925%
31	27.860	4138	4148	4157	rBV4	16295	61153	4.04%	0.790%

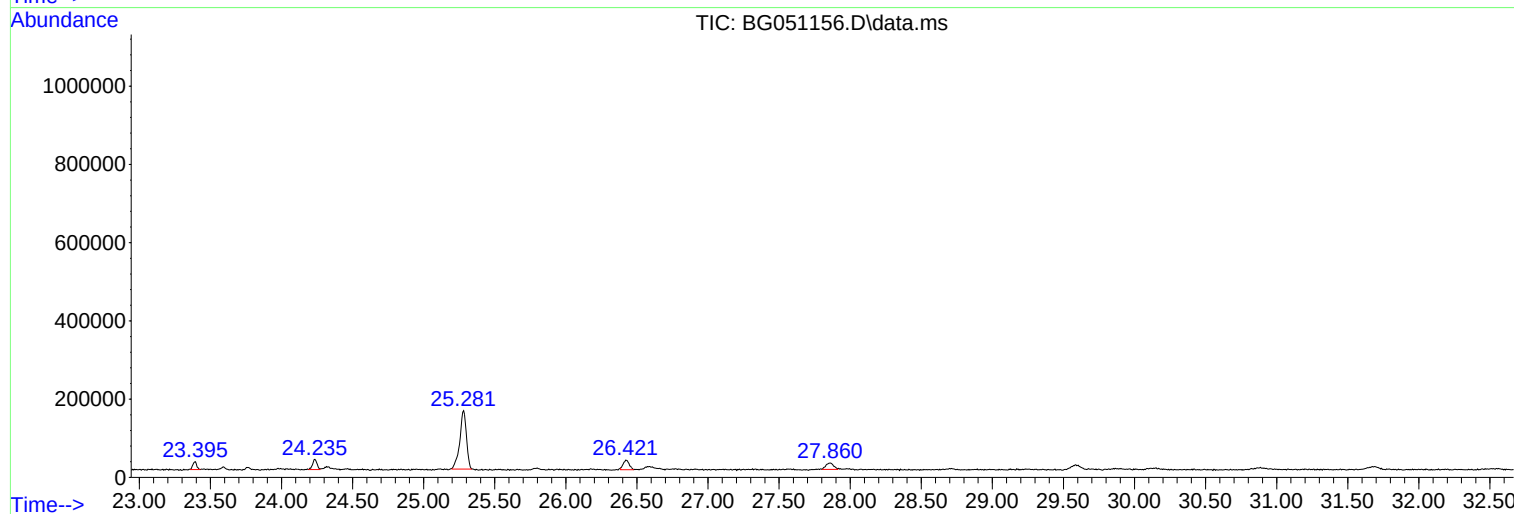
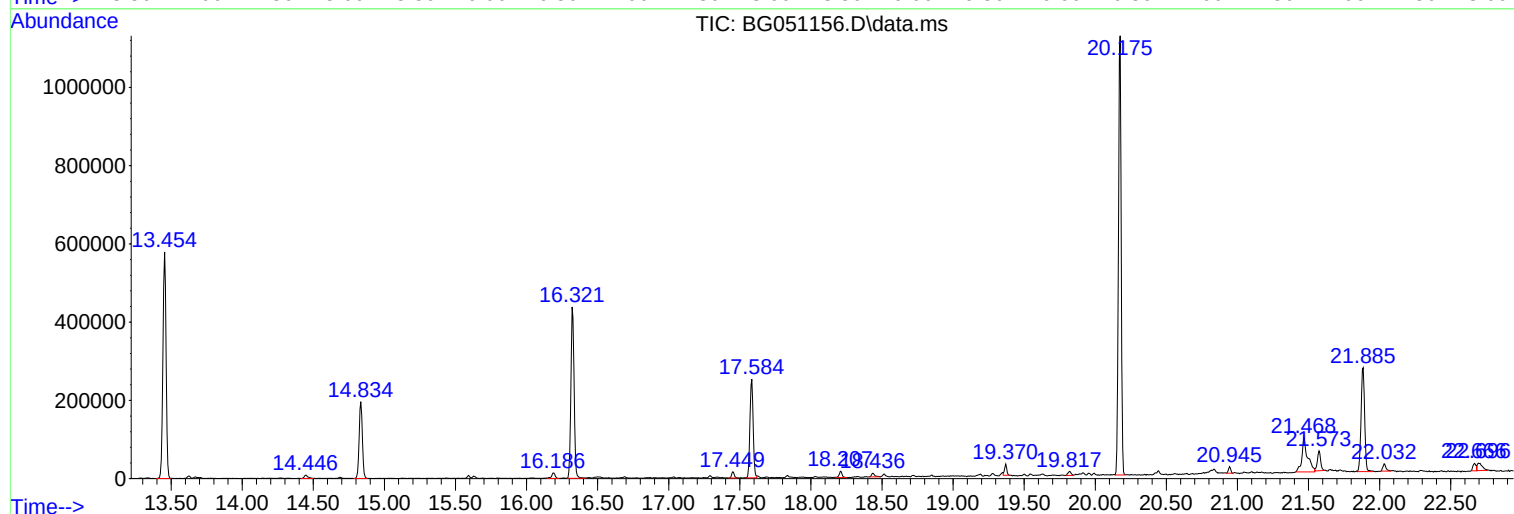
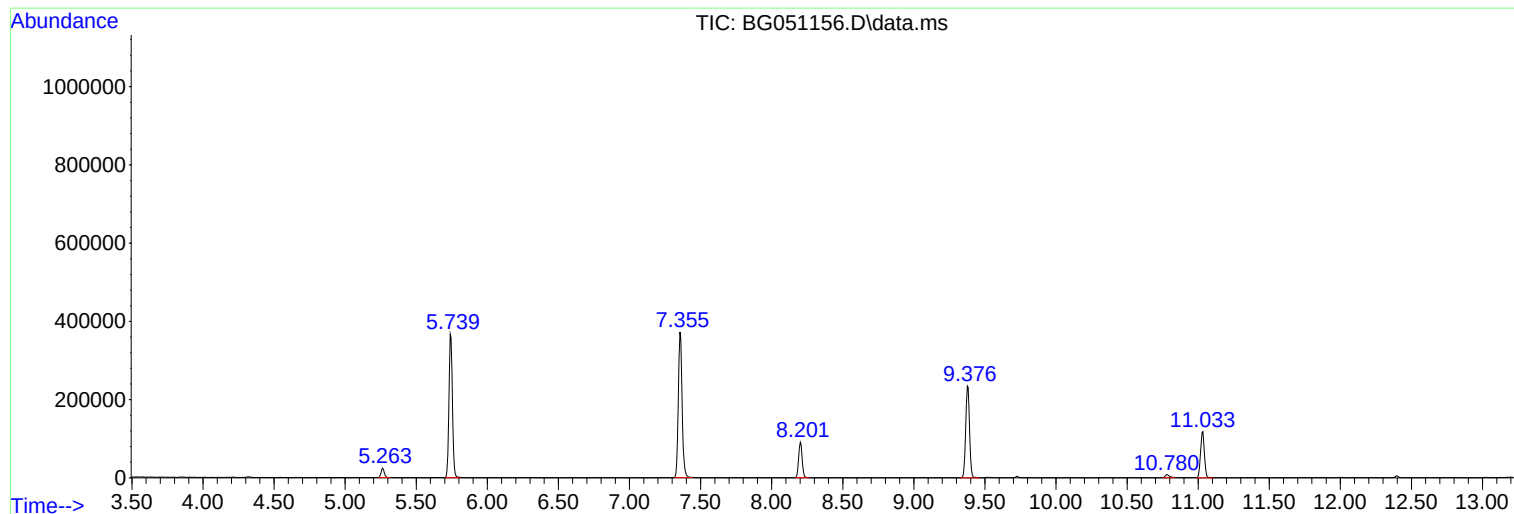
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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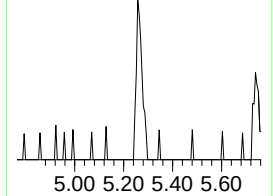
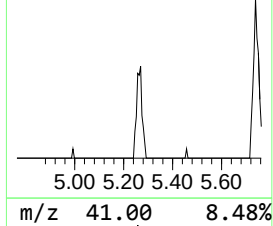
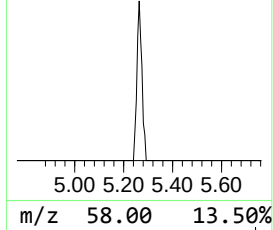
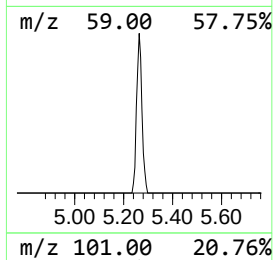
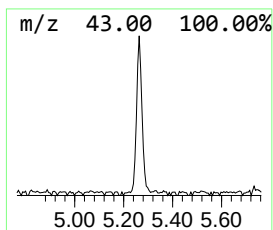
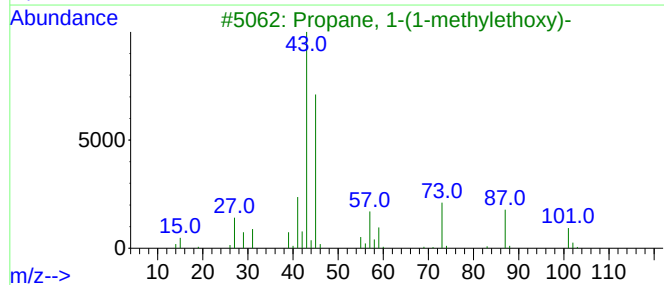
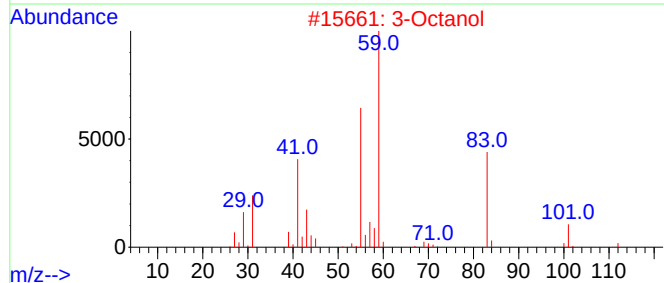
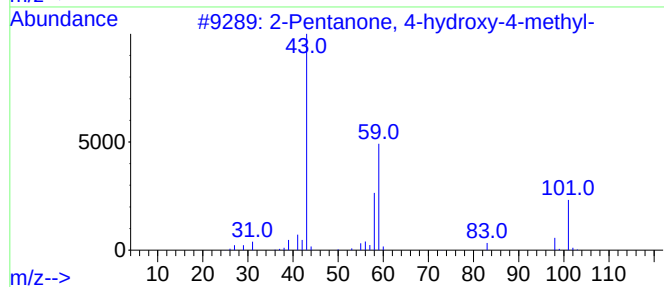
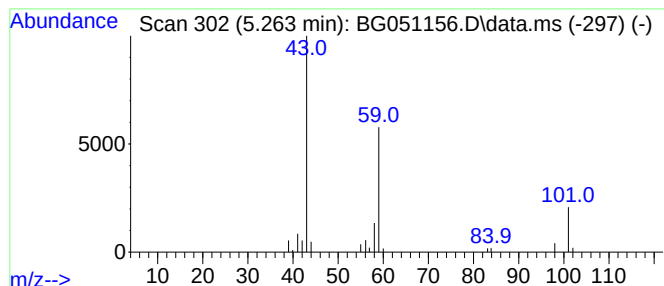
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.263	4.83 ng	37687	1,4-Dichlorobenzene-d4	8.201

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	3-Octanol	130	C8H18O	000589-98-0	23		
3	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	9		
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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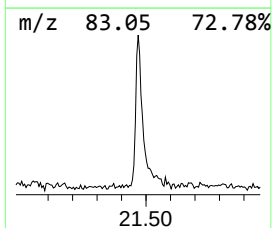
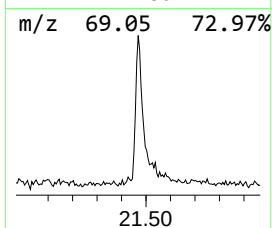
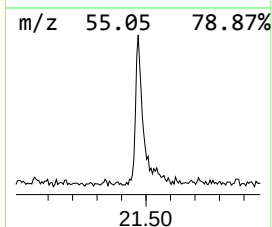
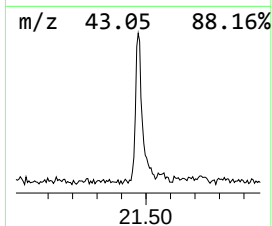
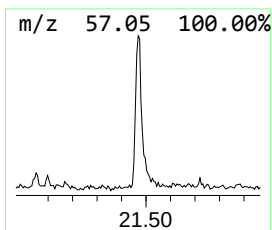
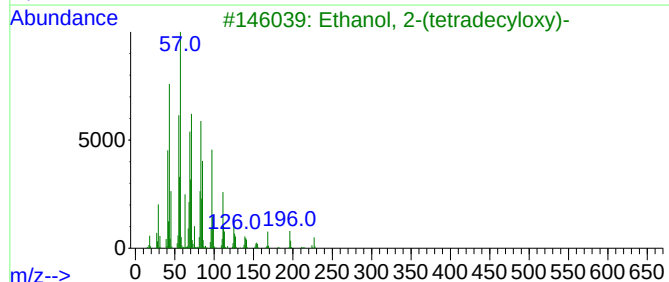
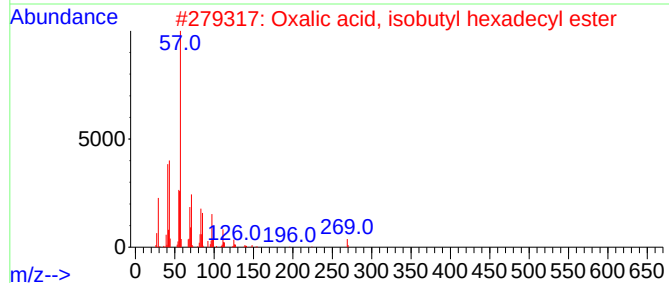
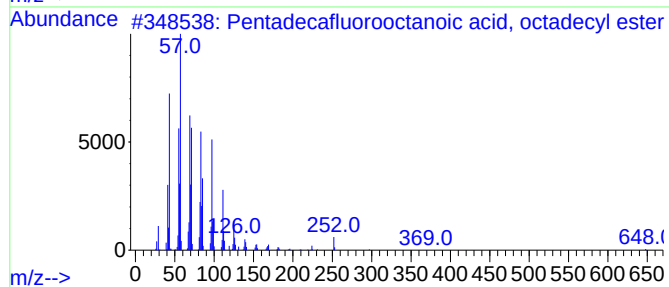
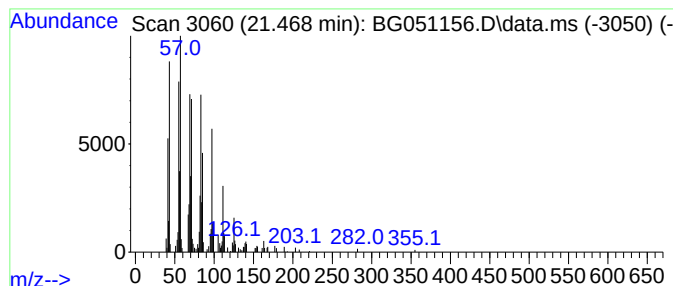
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Peak Number 2 Pentadecafluorooctanoic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.468	10.63 ng	244686	Chrysene-d12	21.885

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
3			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
4			Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	91
5			1-Hexacosene	364	C26H52	018835-33-1	87



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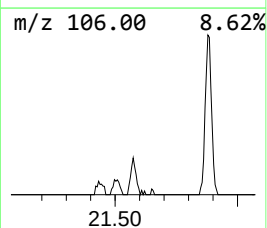
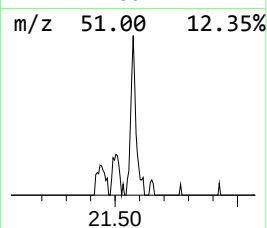
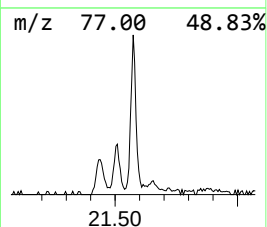
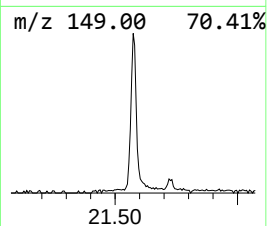
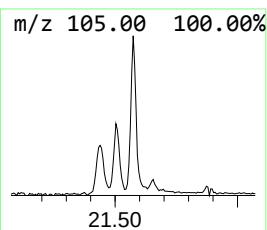
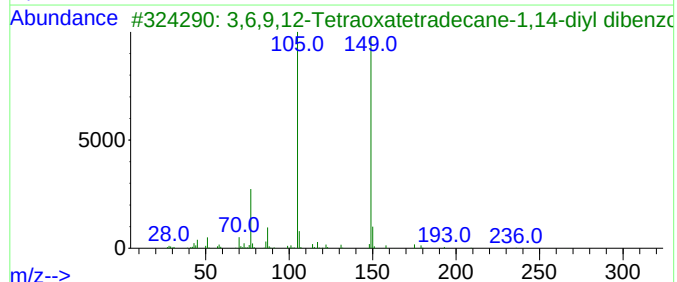
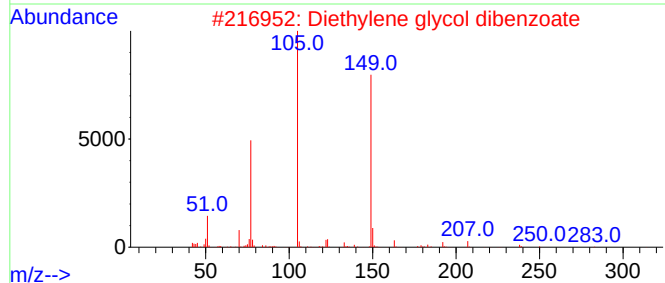
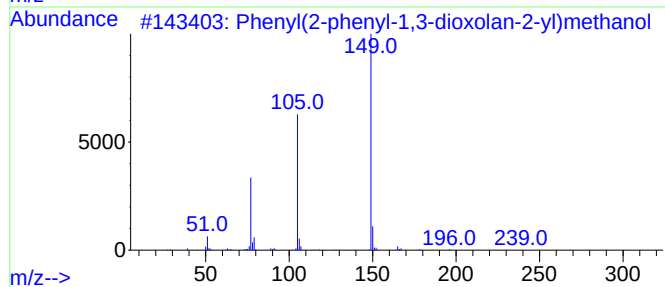
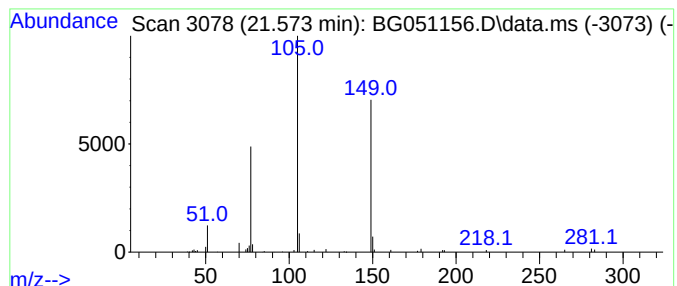
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Phenyl(2-phenyl-1,3-dioxola... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.573	3.44 ng	79178	Chrysene-d12	21.885

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenyl(2-phenyl-1,3-dioxolan-2-y...	256	C16H16O3	005694-69-9	78
2			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	78
3			3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	78
4			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	78
5			Phenyl(2-phenyl-1,3-dioxolan-2-y...	270	C17H18O3	1000507-07-6	78



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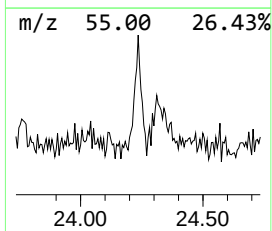
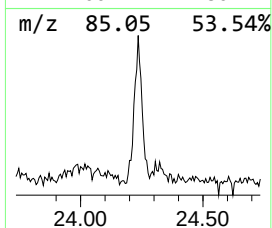
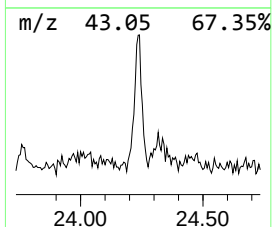
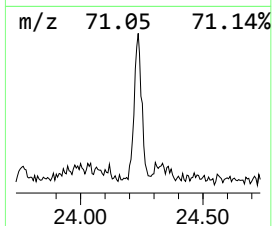
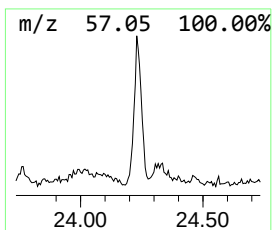
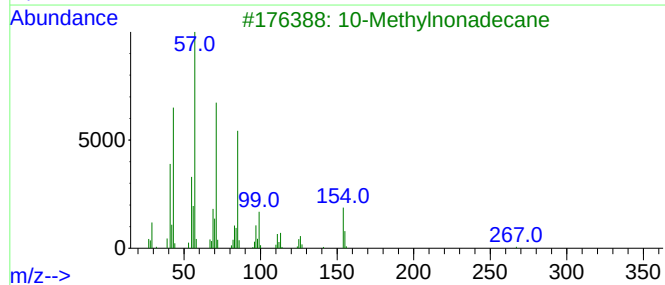
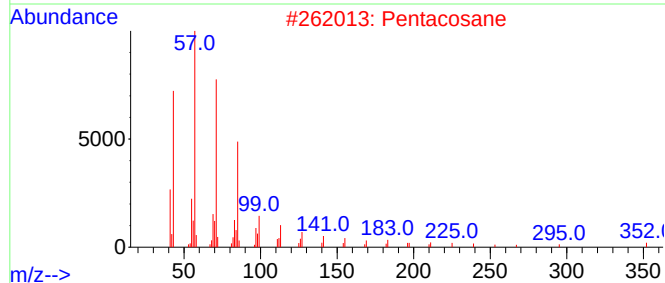
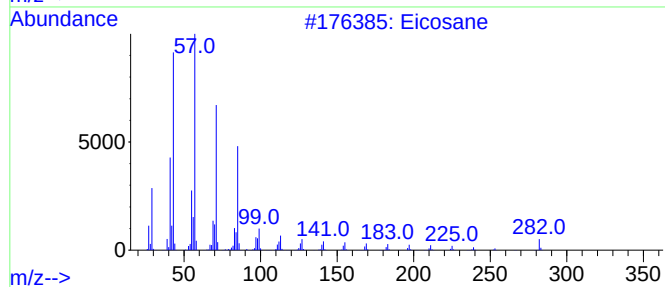
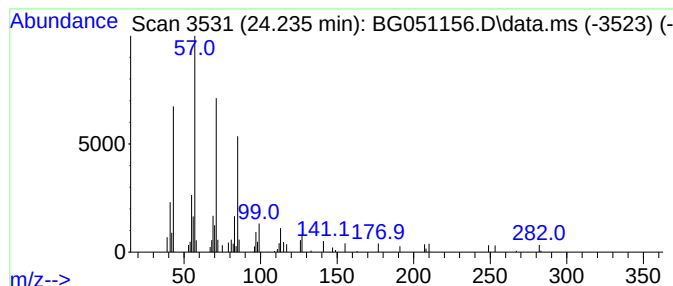
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Peak Number 4 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.235	2.35 ng	57215	Perylene-d12	25.281

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	91
2	Pentacosane			352	C25H52	000629-99-2	90
3	10-Methylnonadecane			282	C20H42	056862-62-5	87
4	Hexacosane			366	C26H54	000630-01-3	87
5	Octadecane			254	C18H38	000593-45-3	86



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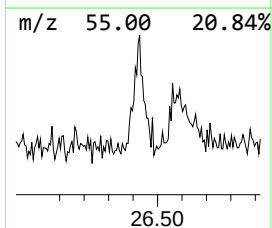
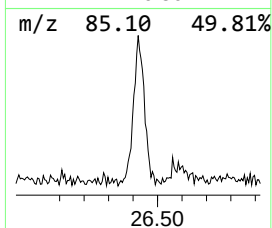
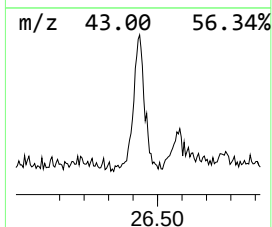
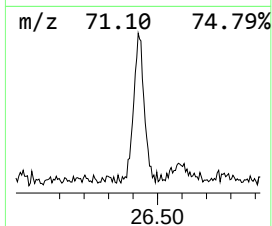
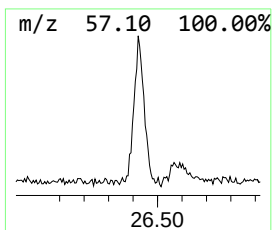
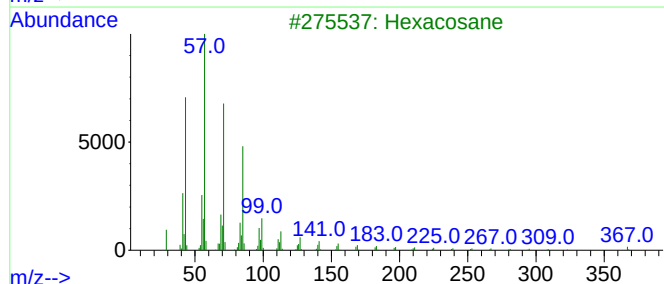
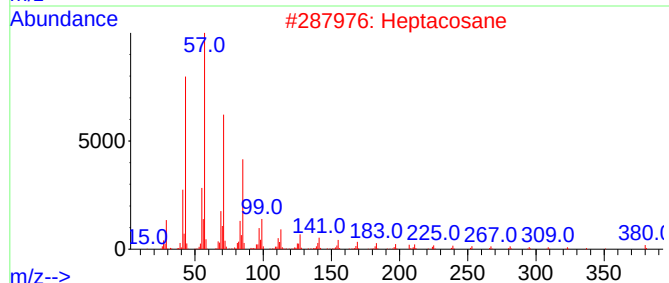
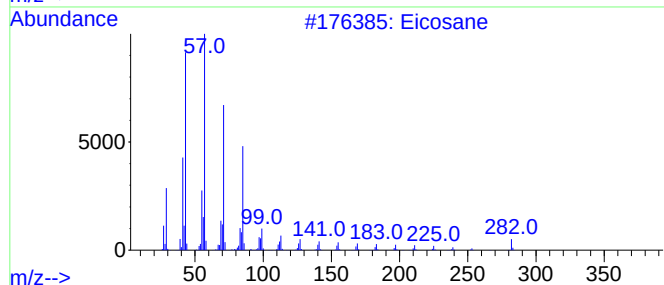
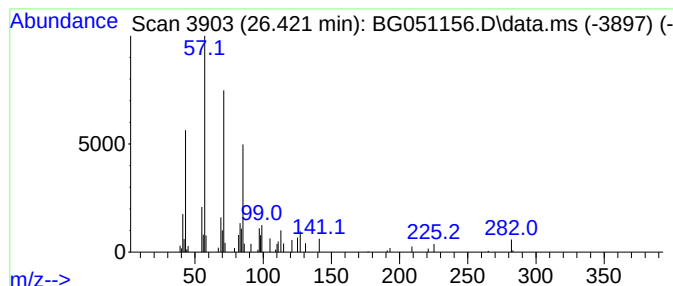
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.421	2.93 ng	71585	Perylene-d12	25.281

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	94
2			Heptacosane	380	C27H56	000593-49-7	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Pentacosane	352	C25H52	000629-99-2	91
5			Hexatriacontane	507	C36H74	000630-06-8	90



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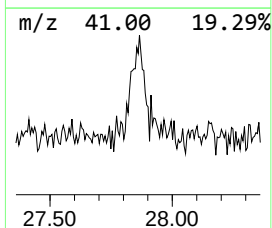
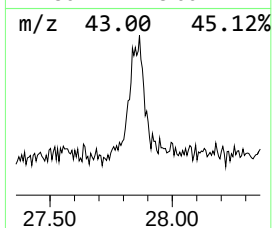
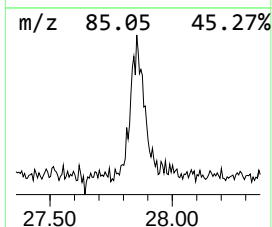
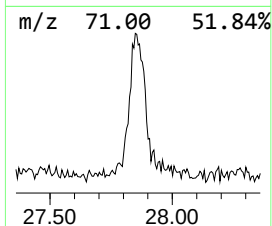
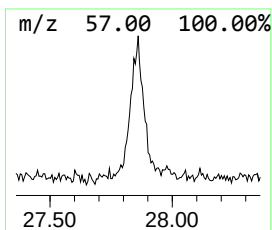
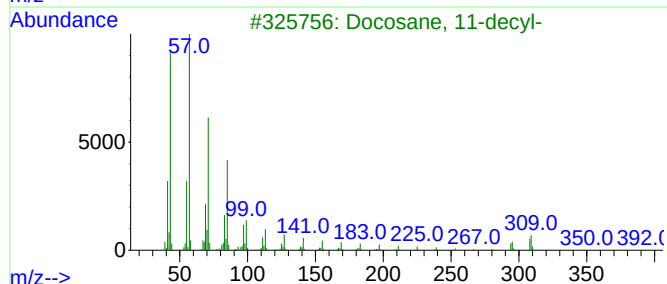
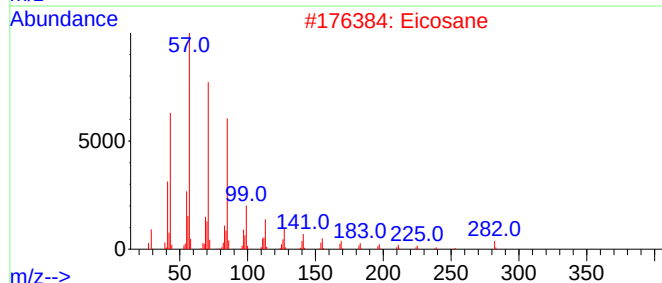
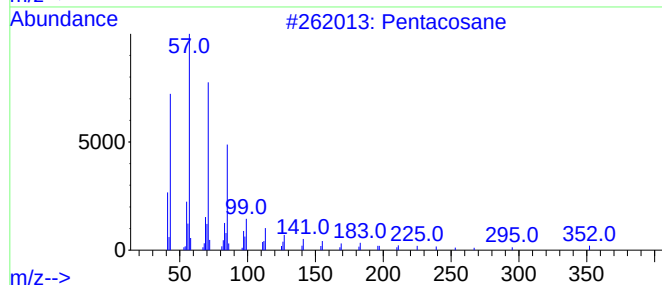
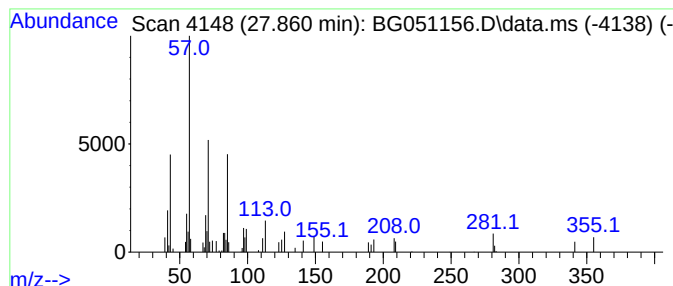
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.860	2.51 ng	61153	Perylene-d12	25.281

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	83
2			Eicosane	282	C20H42	000112-95-8	81
3			Docosane, 11-decyl-	451	C32H66	055401-55-3	80
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	80
5			Tetracosane	338	C24H50	000646-31-1	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112021\
Data File : BG051156.D
Acq On : 20 Nov 2021 20:39
Operator : CG/JU
Sample : M4758-31
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.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
2-Pentanone, 4-...	5.263	4.8	ng	37687	1	8.201	156150	20.0
Pentadecafluoro...	21.468	10.6	ng	244686	5	21.885	460459	20.0
Phenyl(2-phenyl...	21.573	3.4	ng	79178	5	21.885	460459	20.0
Eicosane	24.235	2.4	ng	57215	6	25.281	487942	20.0
Heptacosane	26.421	2.9	ng	71585	6	25.281	487942	20.0
Pentacosane	27.860	2.5	ng	61153	6	25.281	487942	20.0