

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040324\
 Data File : BG060760.D
 Acq On : 3 Apr 2024 13:24
 Operator : MA/JU
 Sample : P1954-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RBR21147

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-BG032924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060760.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.099	9	19	28	rBV2	465474	1176396	26.75%	3.827%
2	3.176	28	32	48	rVB	578304	1079337	24.54%	3.511%
3	3.358	58	63	74	rVB2	23662	51151	1.16%	0.166%
4	3.693	114	120	128	rBV	50856	82294	1.87%	0.268%
5	5.537	426	434	445	rBV	1115832	1772556	40.30%	5.767%
6	7.118	693	703	712	rBV	1100426	1862719	42.35%	6.060%
7	7.958	838	846	854	rBV	295265	490482	11.15%	1.596%
8	9.110	1034	1042	1052	rBV	688027	1203389	27.36%	3.915%
9	10.755	1314	1322	1330	rBV	370582	664083	15.10%	2.160%
10	11.489	1441	1447	1453	rBV3	34795	64728	1.47%	0.211%
11	13.211	1733	1740	1748	rBV	1737280	2653472	60.33%	8.632%
12	14.586	1967	1974	1981	rVB	592943	935888	21.28%	3.045%
13	14.821	2003	2014	2022	rBV	1935043	4344899	98.79%	14.135%
14	16.072	2219	2227	2234	rBV	1417482	2224768	50.58%	7.238%
15	17.330	2435	2441	2447	rBV	812183	1213147	27.58%	3.947%
16	18.029	2555	2560	2566	rVB2	42233	63654	1.45%	0.207%
17	18.240	2591	2596	2604	rBV	358912	524756	11.93%	1.707%
18	18.375	2612	2619	2629	rVB2	55928	180591	4.11%	0.588%
19	19.104	2740	2743	2749	rBV2	32159	49601	1.13%	0.161%
20	19.333	2778	2782	2786	rBV	38079	44520	1.01%	0.145%
21	19.515	2809	2813	2817	rBV	187229	262017	5.96%	0.852%
22	19.574	2817	2823	2832	rVB2	140114	342061	7.78%	1.113%
23	19.956	2882	2888	2895	rBV	3314687	4398090	100.00%	14.308%
24	20.479	2971	2977	2984	rVB	222973	384205	8.74%	1.250%
25	21.284	3108	3114	3124	rBV2	433957	810355	18.43%	2.636%
26	21.595	3161	3167	3173	rVB	855815	1328125	30.20%	4.321%
27	22.189	3262	3268	3275	rVB	199613	416095	9.46%	1.354%
28	23.223	3438	3444	3455	rVB2	143428	381387	8.67%	1.241%
29	24.415	3642	3647	3659	rVB3	102800	302254	6.87%	0.983%
30	24.733	3693	3701	3715	rVB	488002	1431387	32.55%	4.657%

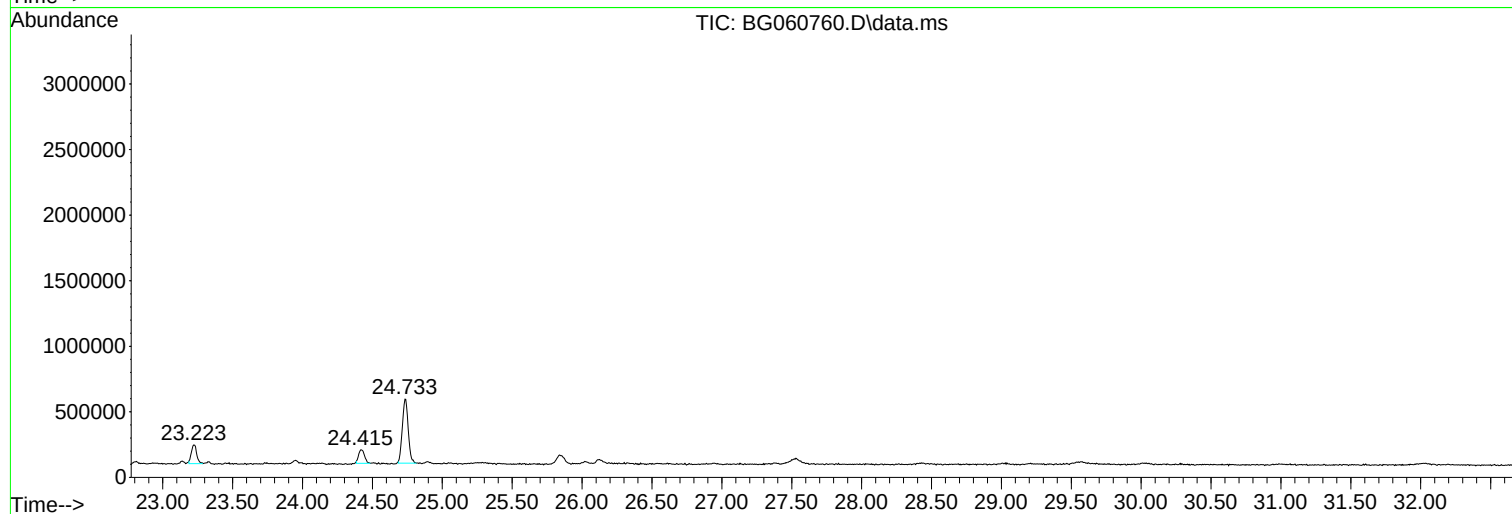
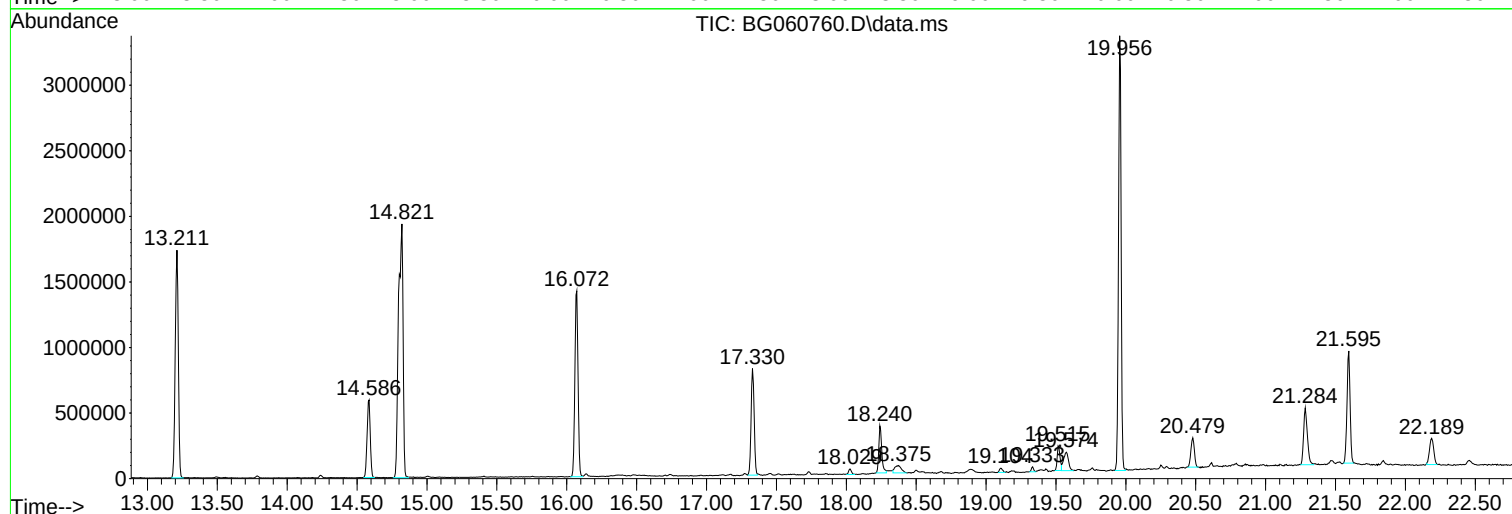
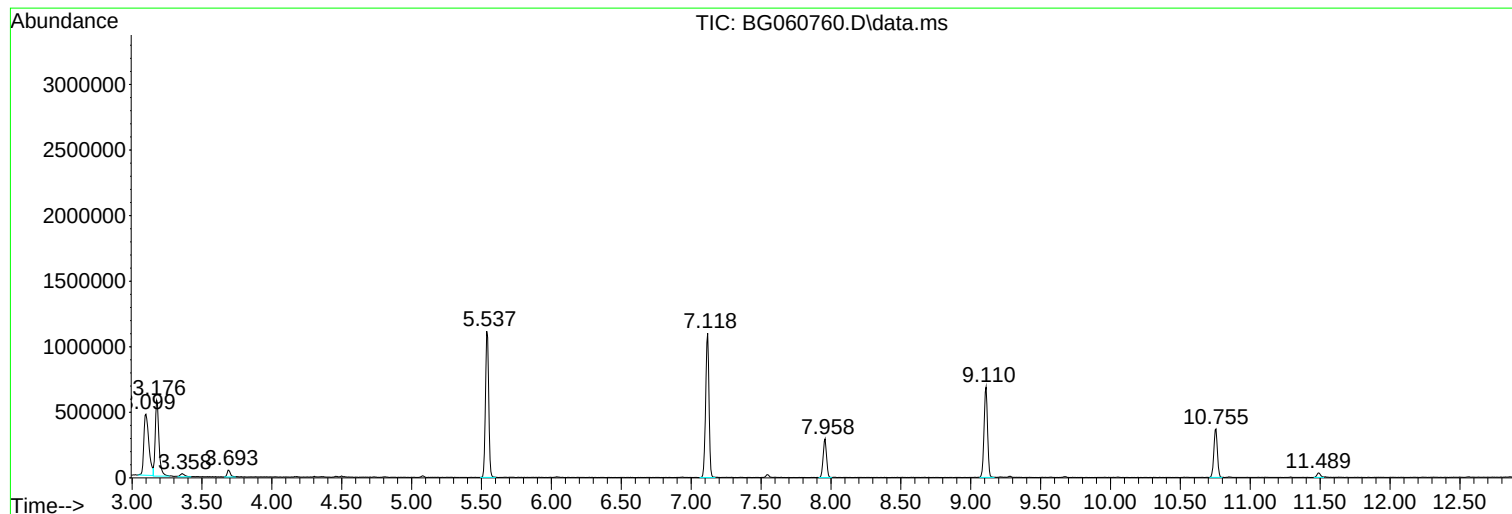
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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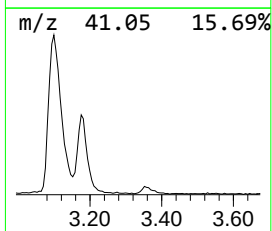
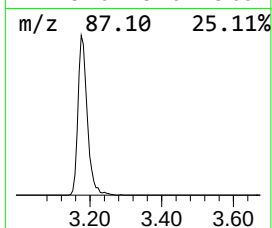
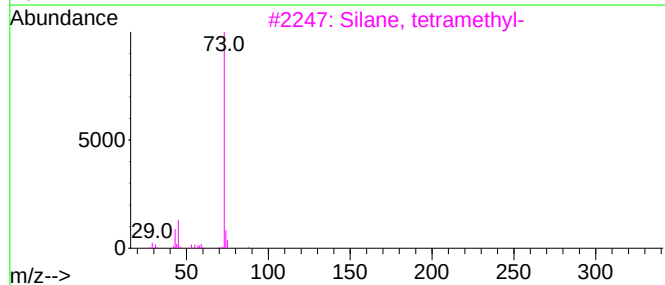
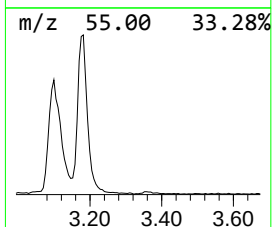
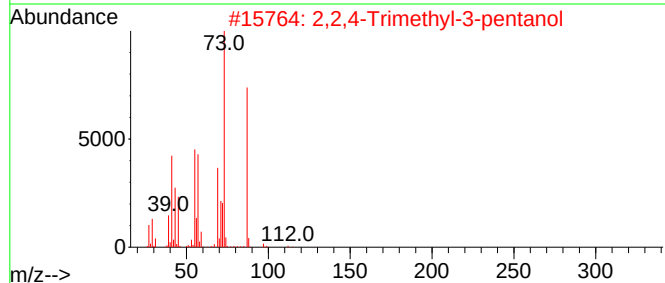
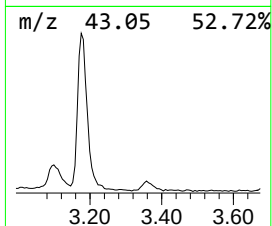
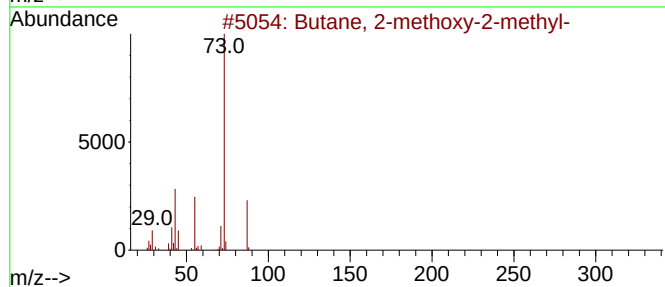
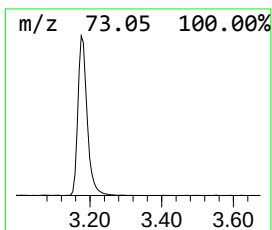
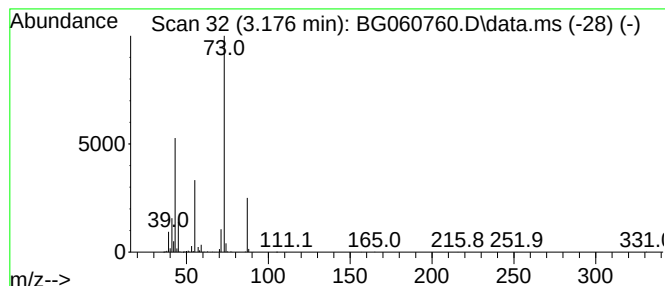
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.176	44.01 ng	1079340	1,4-Dichlorobenzene-d4	7.958

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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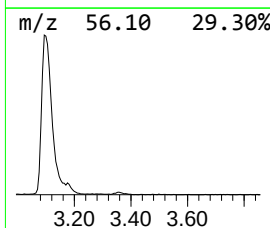
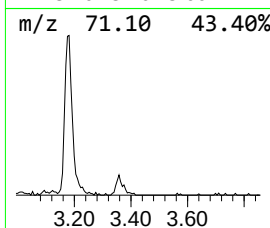
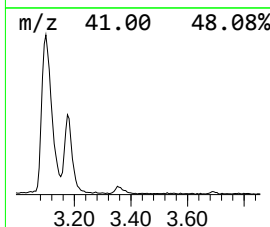
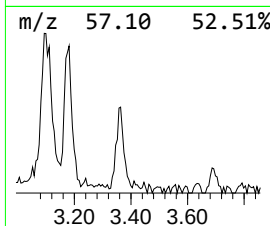
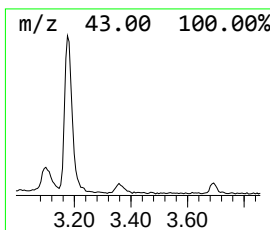
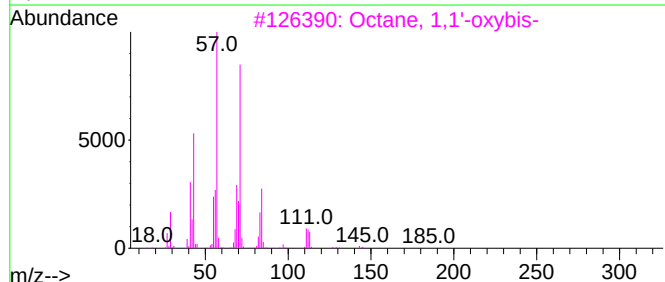
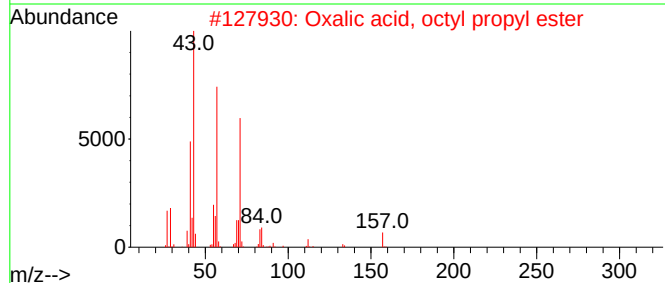
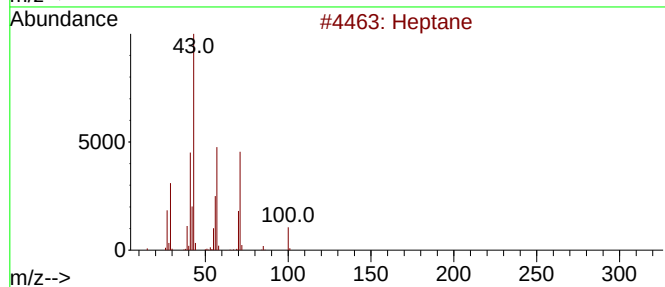
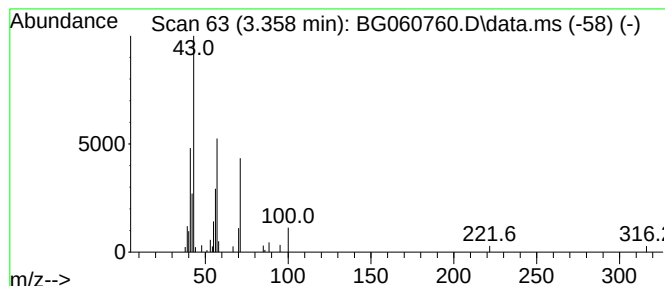
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Heptane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.358	2.09 ng	51151	1,4-Dichlorobenzene-d4	7.958

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	83
2			Oxalic acid, octyl propyl ester	244	C13H24O4	1010309-26-1	42
3			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	37
4			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	37
5			Hexane, 3-methyl-	100	C7H16	000589-34-4	36



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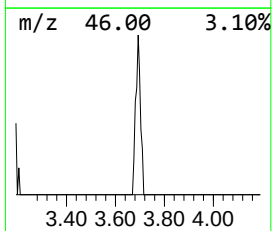
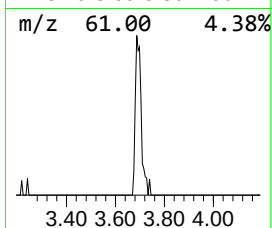
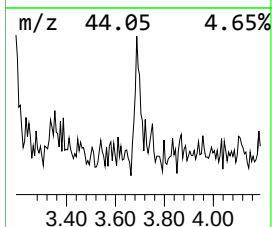
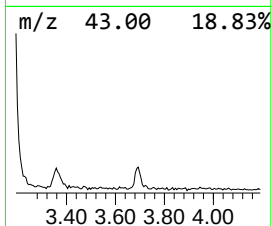
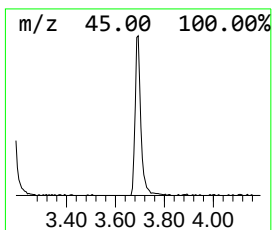
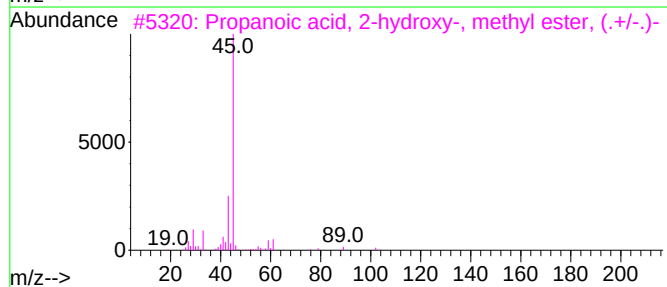
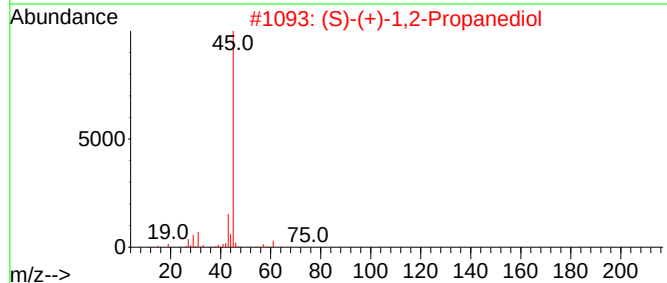
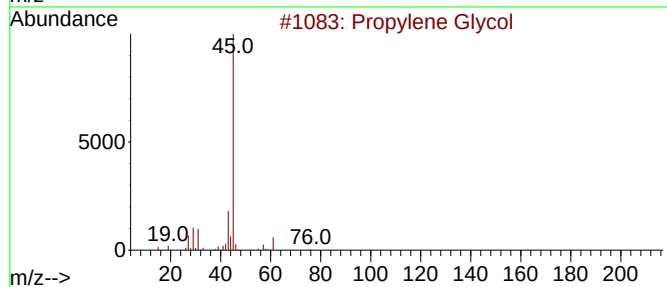
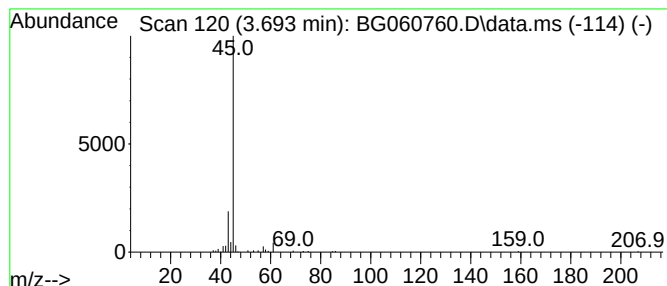
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Propylene Glycol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.693	3.36 ng	82294	1,4-Dichlorobenzene-d4	7.958

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	56
2			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	39
3			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
4			2-Hexanol	102	C6H14O	000626-93-7	9
5			Formamide	45	CH3NO	000075-12-7	7



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ALS Vial : 6 Sample Multiplier: 1

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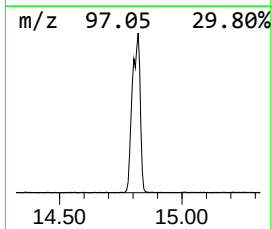
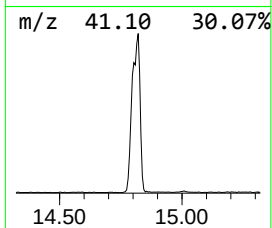
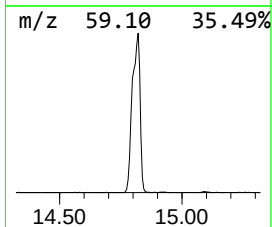
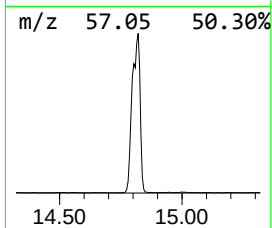
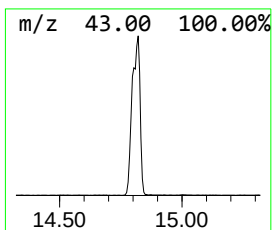
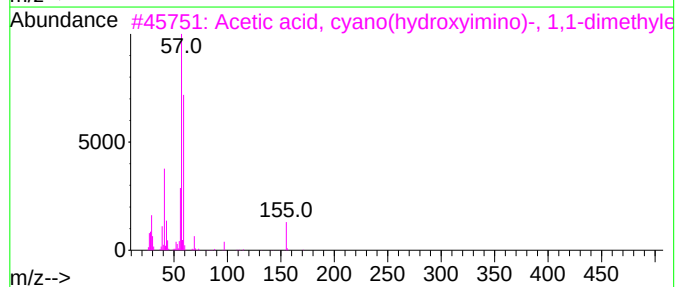
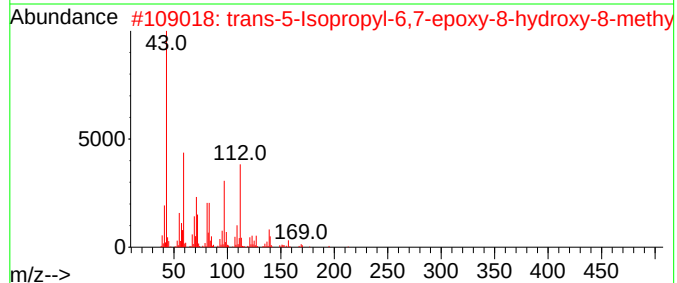
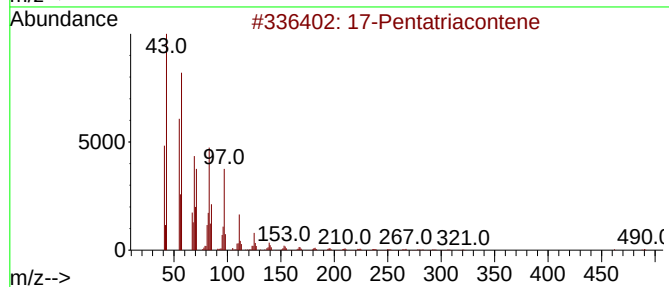
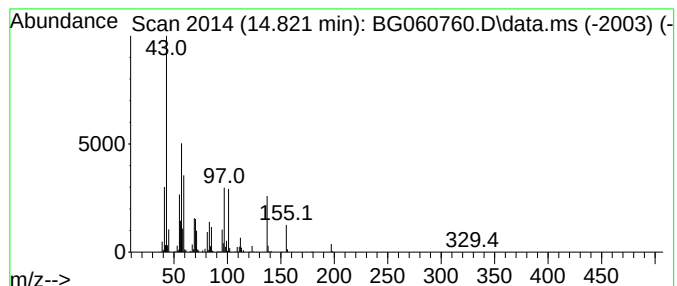
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown14.821 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.821	92.85 ng	4344900	Acenaphthene-d10	14.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	10
2			trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	10
3			Acetic acid, cyano(hydroxyimino)...	170	C7H10N2O3	076101-98-9	10
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	10
5			Pentadecane, 1-bromo-	290	C15H31Br	000629-72-1	10



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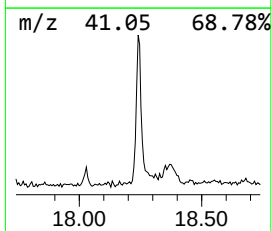
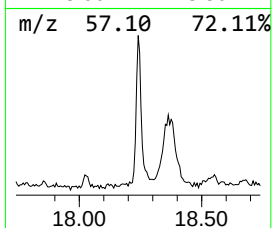
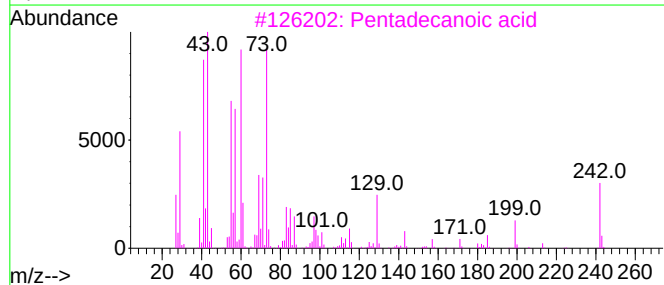
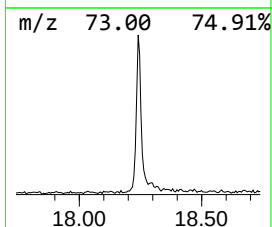
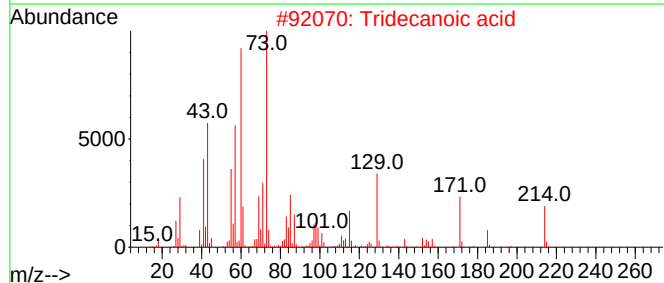
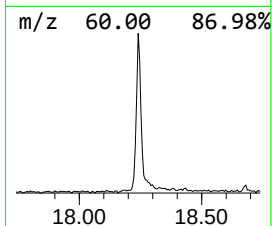
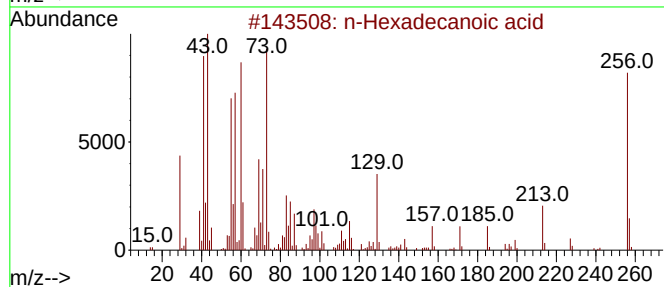
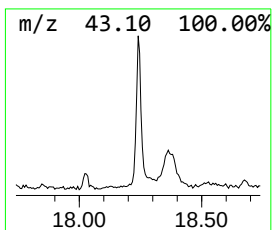
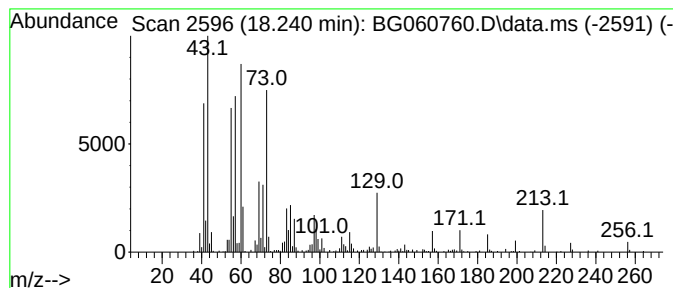
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.240	8.65 ng	524756	Phenanthrene-d10	17.329	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Tridecanoic acid	214	C13H26O2	000638-53-9	72
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Isopropyl palmitate	298	C19H38O2	000142-91-6	64



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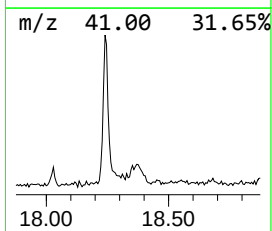
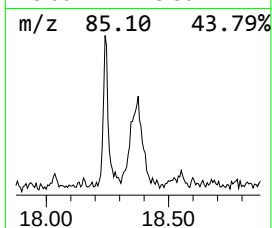
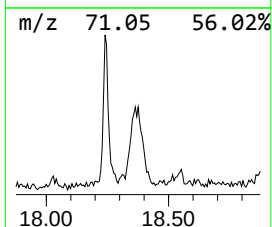
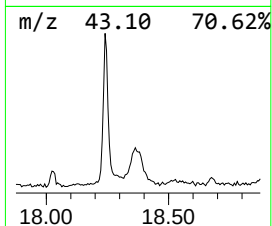
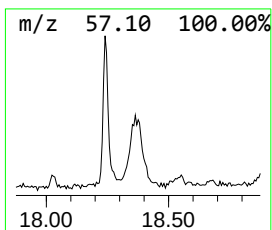
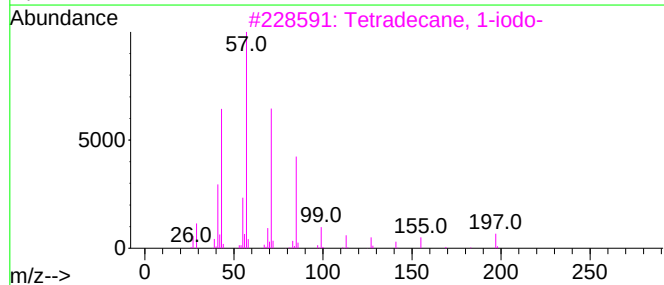
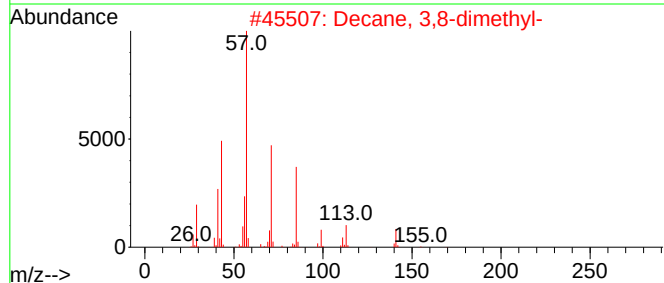
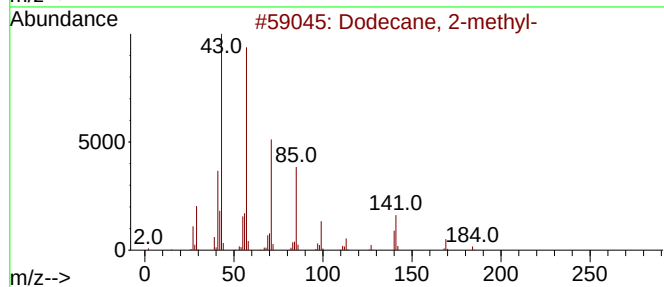
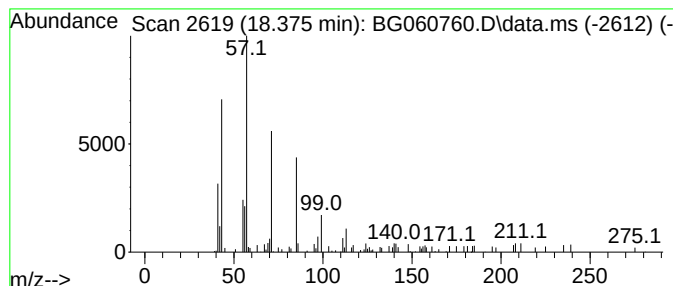
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Dodecane, 2-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.375	2.98 ng	180591	Phenanthrene-d10	17.329

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2-methyl-	184	C13H28	001560-97-0	87
2			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	72
3			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	64
4			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	64
5			Undecane, 3,7-dimethyl-	184	C13H28	017301-29-0	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040324\
Data File : BG060760.D
Acq On : 3 Apr 2024 13:24
Operator : MA/JU
Sample : P1954-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

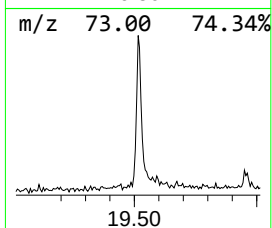
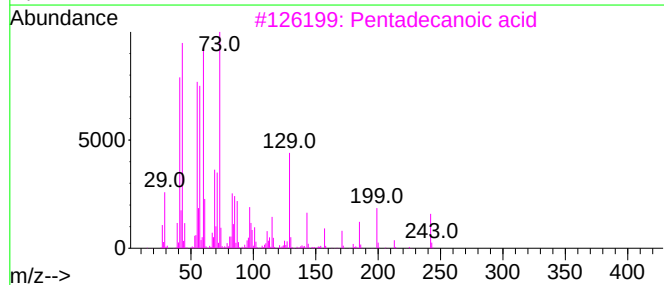
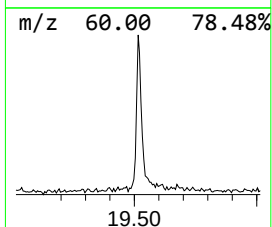
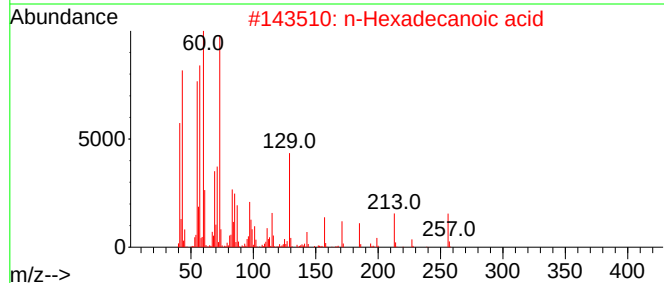
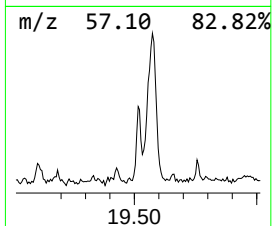
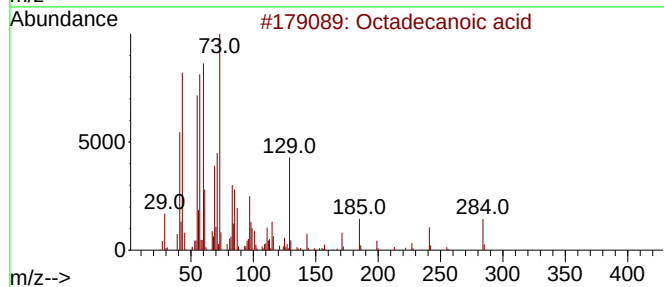
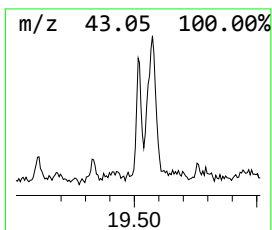
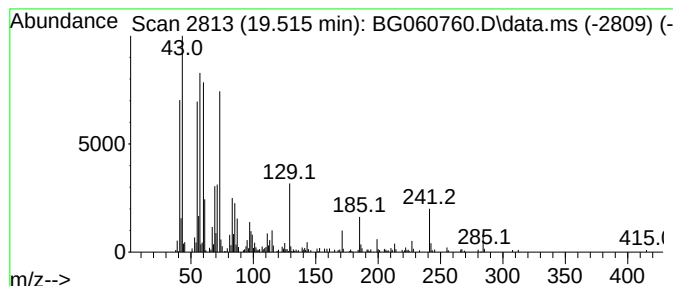
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.515	3.95 ng	262017	Chrysene-d12		21.595	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octadecanoic acid		284	C18H36O2	000057-11-4	95
2	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	80
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	74
4	Undecanoic acid		186	C11H22O2	000112-37-8	62
5	n-Decanoic acid		172	C10H20O2	000334-48-5	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040324\
Data File : BG060760.D
Acq On : 3 Apr 2024 13:24
Operator : MA/JU
Sample : P1954-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

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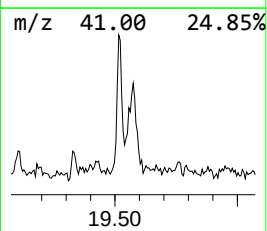
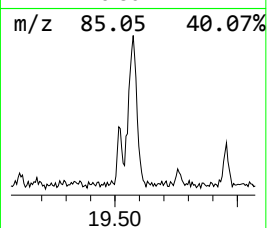
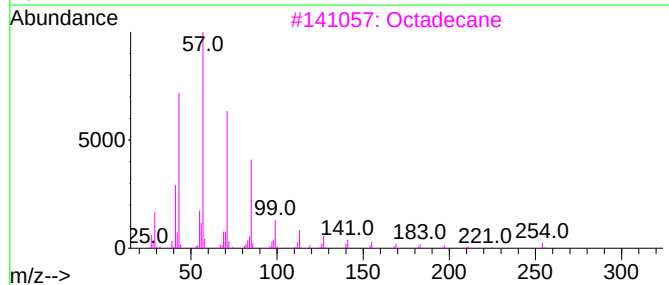
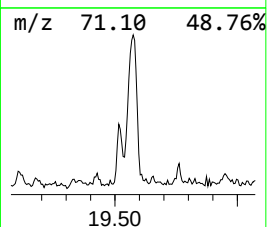
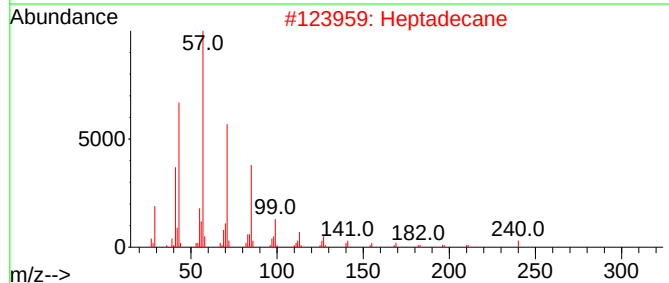
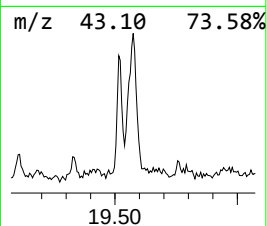
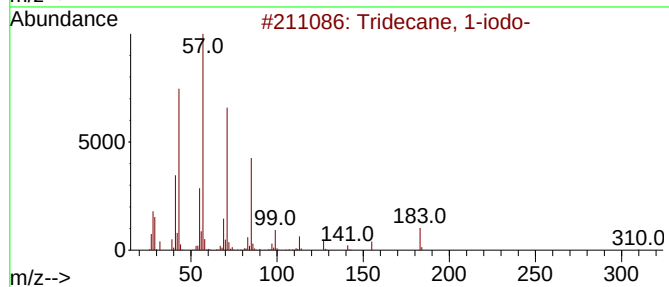
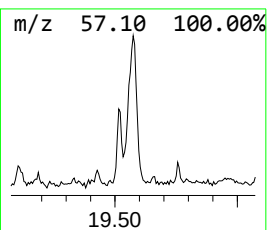
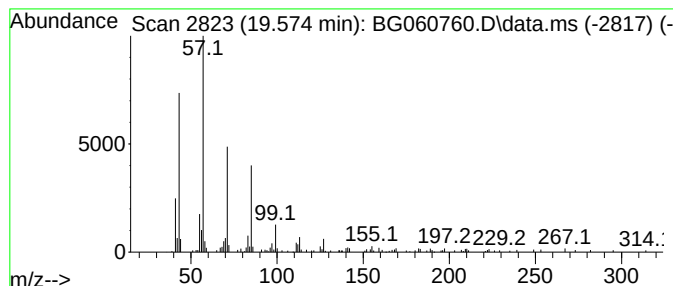
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tridecane, 1-iodo- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.574	5.15 ng	342061	Chrysene-d12	21.595

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87
2			Heptadecane	240	C17H36	000629-78-7	83
3			Octadecane	254	C18H38	000593-45-3	78
4			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	72
5			2-Bromo dodecane	248	C12H25Br	013187-99-0	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040324\
Data File : BG060760.D
Acq On : 3 Apr 2024 13:24
Operator : MA/JU
Sample : P1954-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

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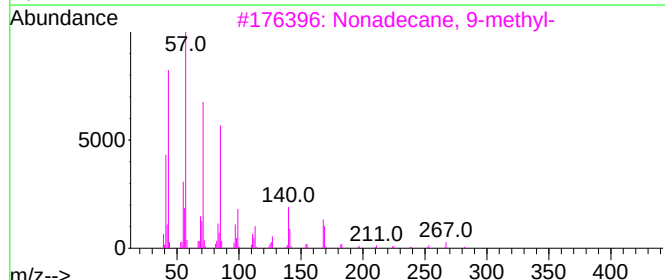
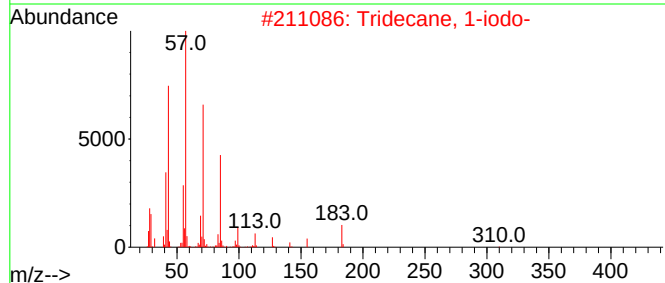
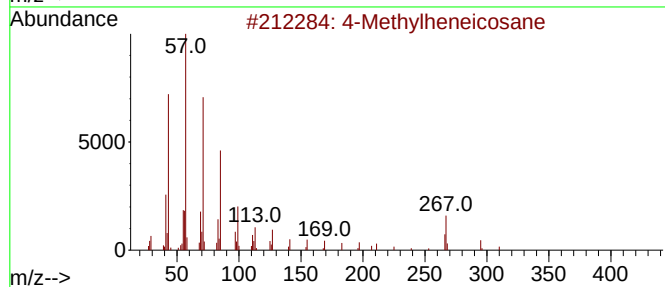
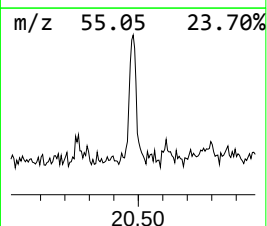
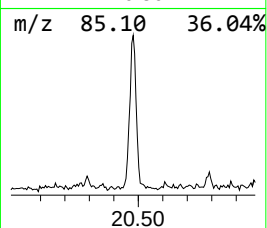
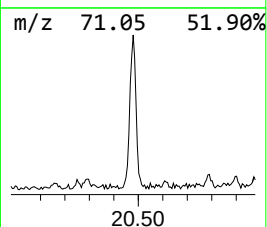
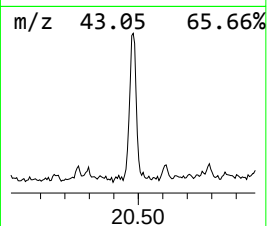
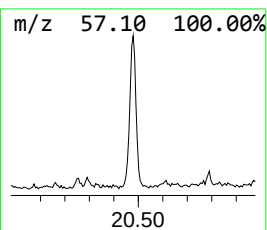
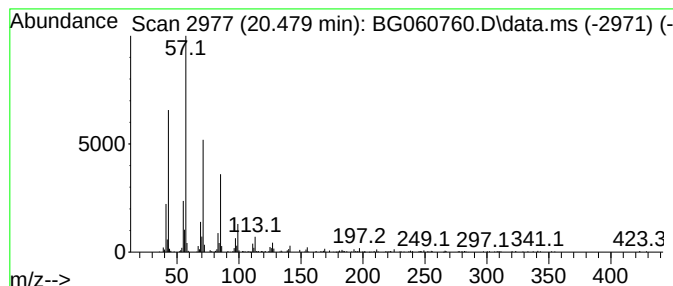
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 4-Methylheneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.479	5.79 ng	384205	Chrysene-d12	21.595

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Methylheneicosane	310	C22H46	025117-29-7	95
2		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	93
3		Nonadecane, 9-methyl-	282	C20H42	013287-24-6	91
4		Heptacosane	380	C27H56	000593-49-7	91
5		Hentriacontane	437	C31H64	000630-04-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040324\
Data File : BG060760.D
Acq On : 3 Apr 2024 13:24
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Sample : P1954-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

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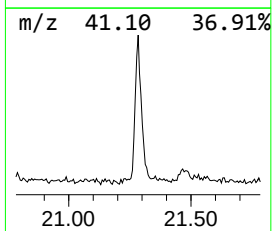
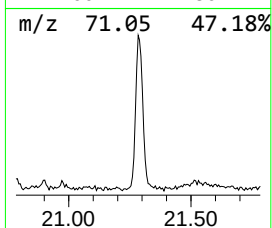
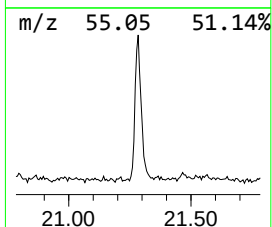
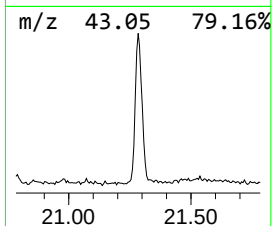
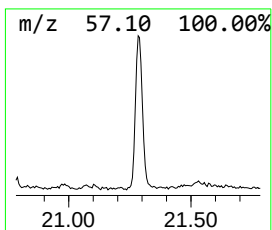
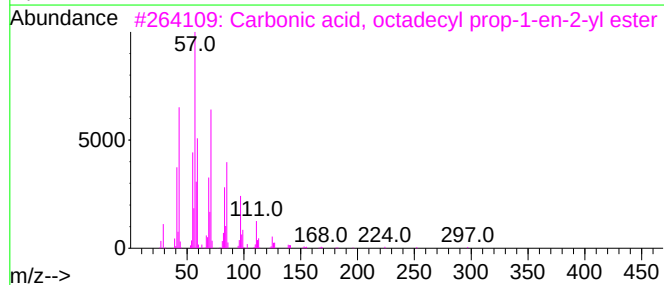
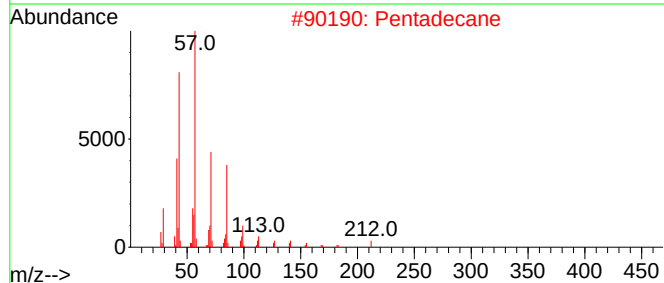
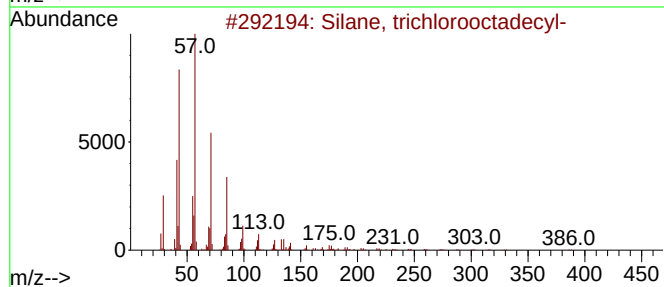
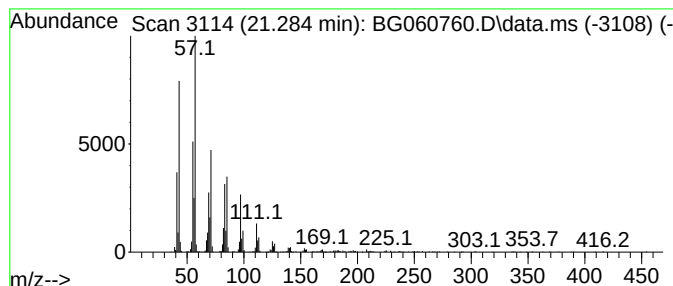
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Silane, trichlorooctadecyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.284	12.20 ng	810355	Chrysene-d12	21.595

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	92
2			Pentadecane	212	C15H32	000629-62-9	91
3			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	90
4			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	87
5			Cyclotetradecane	196	C14H28	000295-17-0	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040324\
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Misc :
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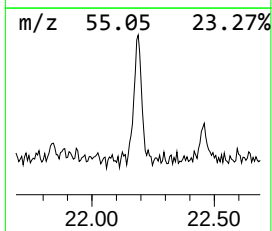
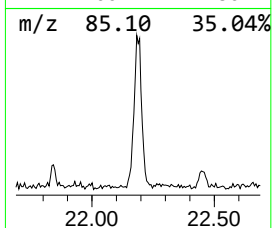
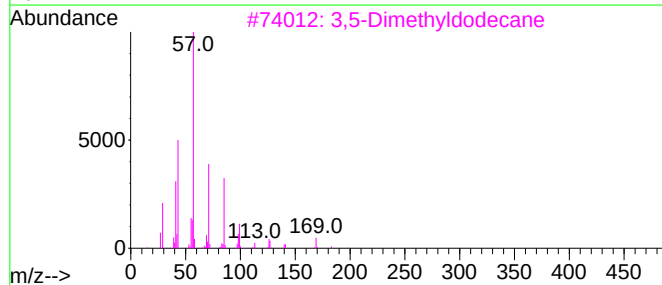
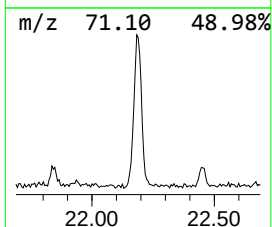
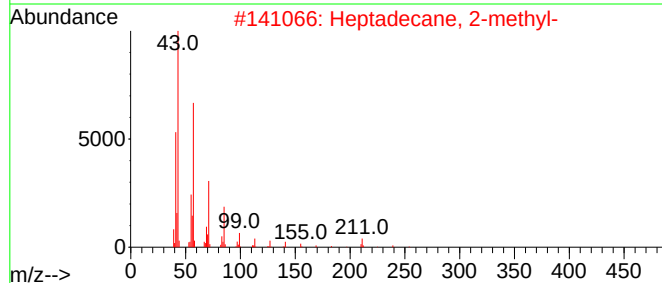
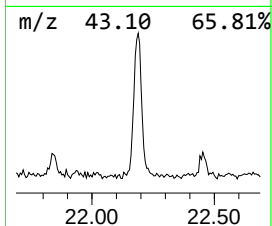
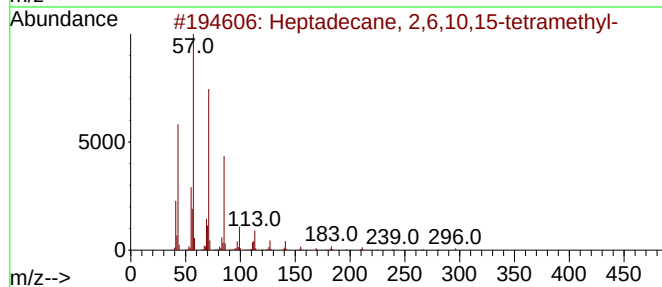
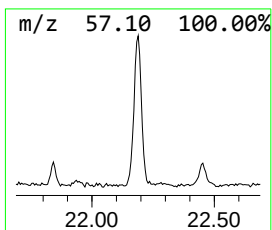
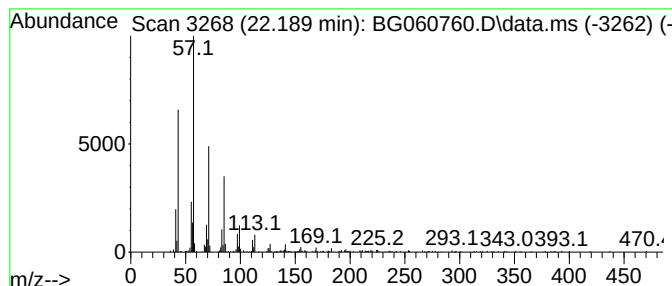
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heptadecane, 2,6,10,15-tetr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.189	6.27 ng	416095	Chrysene-d12	21.595	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	95
2	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	87
3	3,5-Dimethyldodecane	198	C14H30	107770-99-0	83
4	Eicosane	282	C20H42	000112-95-8	83
5	Nonadecane	268	C19H40	000629-92-5	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040324\
Data File : BG060760.D
Acq On : 3 Apr 2024 13:24
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Sample : P1954-01
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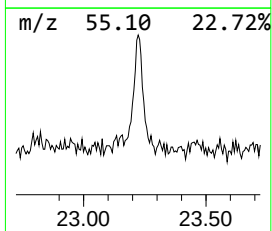
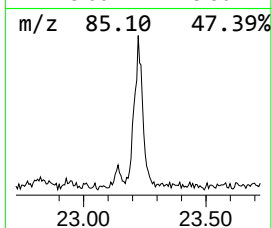
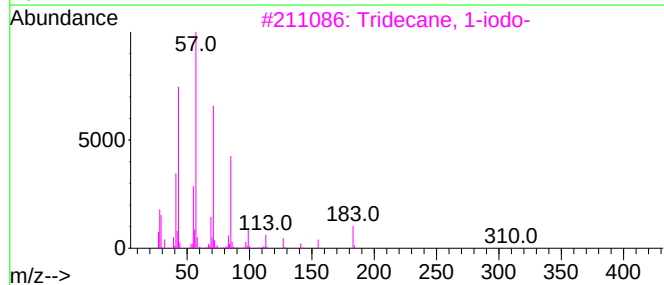
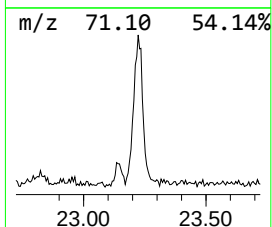
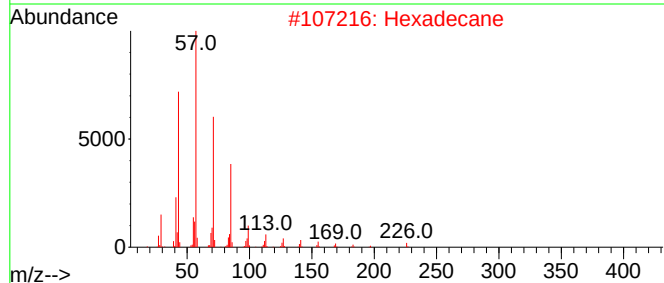
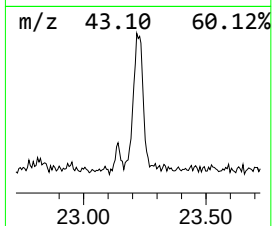
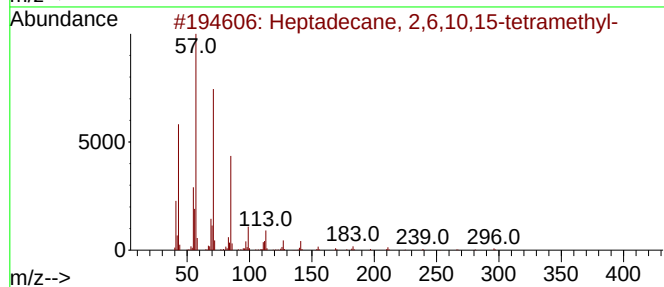
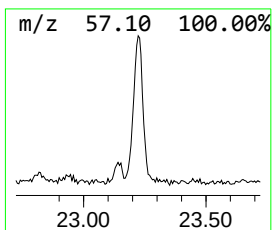
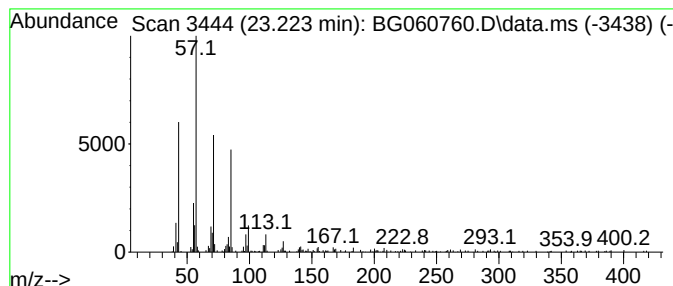
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.223	5.33 ng	381387	Perylene-d12	24.738

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
2		Hexadecane	226	C16H34	000544-76-3	80
3		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80
4		Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	72
5		Heneicosane	296	C21H44	000629-94-7	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040324\
Data File : BG060760.D
Acq On : 3 Apr 2024 13:24
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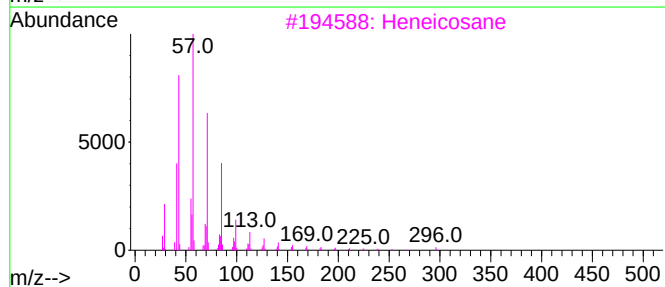
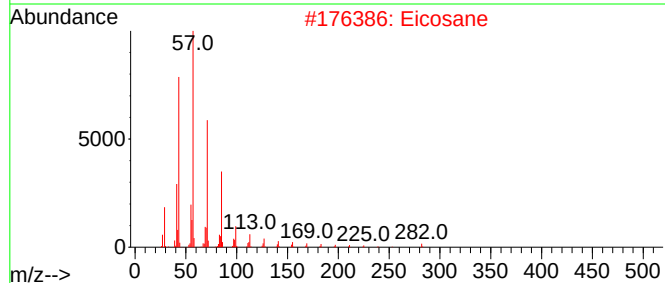
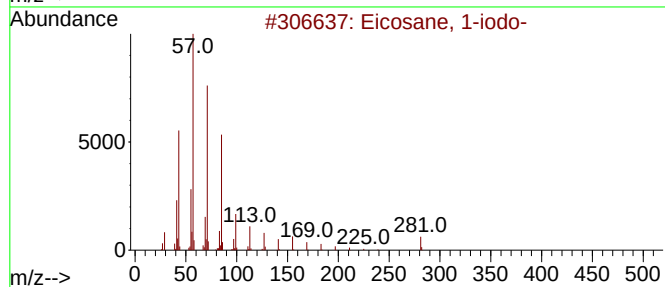
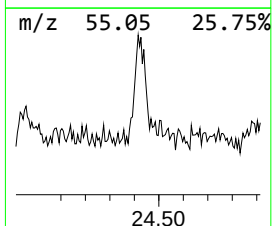
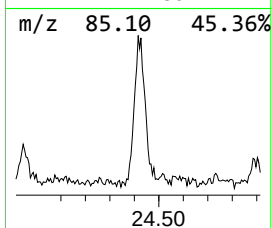
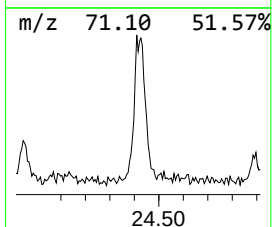
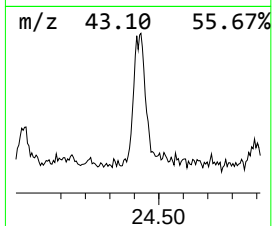
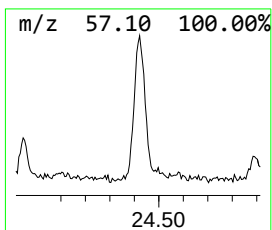
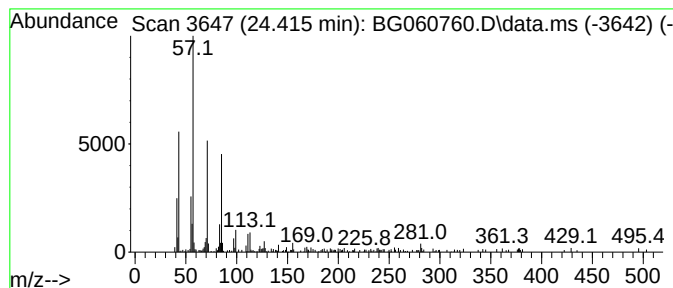
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Eicosane, 1-iodo- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.415	4.22 ng	302254	Perylene-d12	24.738

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	80
2			Eicosane	282	C20H42	000112-95-8	78
3			Heneicosane	296	C21H44	000629-94-7	78
4			Hexadecane	226	C16H34	000544-76-3	74
5			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040324\
Data File : BG060760.D
Acq On : 3 Apr 2024 13:24
Operator : MA/JU
Sample : P1954-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR21147

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.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
Butane, 2-metho...	3.176	44.0	ng	1079340	1	7.958	490482	20.0
Heptane	3.358	2.1	ng	51151	1	7.958	490482	20.0
Propylene Glycol	3.693	3.4	ng	82294	1	7.958	490482	20.0
unknown14.821	14.821	92.8	ng	4344900	3	14.586	935888	20.0
n-Hexadecanoic ...	18.240	8.7	ng	524756	4	17.329	1213150	20.0
Dodecane, 2-met...	18.375	3.0	ng	180591	4	17.329	1213150	20.0
Octadecanoic acid	19.515	4.0	ng	262017	5	21.595	1328130	20.0
Tridecane, 1-iodo-	19.574	5.2	ng	342061	5	21.595	1328130	20.0
4-Methylheneico...	20.479	5.8	ng	384205	5	21.595	1328130	20.0
Silane, trichlo...	21.284	12.2	ng	810355	5	21.595	1328130	20.0
Heptadecane, 2,...	22.189	6.3	ng	416095	5	21.595	1328130	20.0
Hexadecane	23.223	5.3	ng	381387	6	24.738	1431390	20.0
Eicosane, 1-iodo-	24.415	4.2	ng	302254	6	24.738	1431390	20.0