

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042324\
 Data File : BG061012.D
 Acq On : 23 Apr 2024 17:57
 Operator : MA/JU
 Sample : P2227-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 HD-02-04222024

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-BG042024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG061012.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.170	26	31	40	rVB2	20000	43345	2.58%	0.480%
2	3.687	113	119	128	rBV	18574	32899	1.96%	0.364%
3	5.538	427	434	442	rBV	371109	599857	35.76%	6.636%
4	7.112	694	702	711	rBV	374261	630247	37.57%	6.972%
5	7.941	836	843	850	rBV	109138	181933	10.85%	2.013%
6	9.092	1032	1039	1047	rVB	232995	415186	24.75%	4.593%
7	10.738	1311	1319	1328	rBV	139112	251004	14.96%	2.777%
8	11.472	1438	1444	1449	rBV2	9606	17269	1.03%	0.191%
9	13.193	1730	1737	1745	rVB	671410	1001884	59.72%	11.083%
10	14.568	1964	1971	1977	rBV	239784	365844	21.81%	4.047%
11	14.780	2000	2007	2008	rBV3	11746	19553	1.17%	0.216%
12	16.055	2217	2224	2231	rBV	636049	963791	57.45%	10.662%
13	17.312	2432	2438	2443	rBV	288018	460608	27.46%	5.096%
14	17.359	2443	2446	2451	rVB	65263	87004	5.19%	0.962%
15	17.447	2456	2461	2466	rVB2	15200	25425	1.52%	0.281%
16	17.706	2501	2505	2509	rBV4	11822	18974	1.13%	0.210%
17	18.000	2550	2555	2559	rBV	31805	38817	2.31%	0.429%
18	18.217	2583	2592	2602	rBV3	103428	177483	10.58%	1.963%
19	18.387	2615	2621	2625	rBV2	17433	30404	1.81%	0.336%
20	18.522	2638	2644	2647	rBV4	12996	20186	1.20%	0.223%
21	18.646	2661	2665	2669	rBV6	17919	22718	1.35%	0.251%
22	19.134	2744	2748	2751	rBV2	63619	77419	4.62%	0.856%
23	19.169	2751	2754	2758	rVB2	54884	65679	3.92%	0.727%
24	19.298	2773	2776	2782	rVB3	31012	36091	2.15%	0.399%
25	19.369	2782	2788	2793	rBV	165786	240758	14.35%	2.663%
26	19.492	2806	2809	2813	rBV3	35428	44311	2.64%	0.490%
27	19.733	2841	2850	2858	rVB	132818	233378	13.91%	2.582%
28	19.938	2877	2885	2890	rBV	1323302	1677508	100.00%	18.558%
29	20.226	2930	2934	2937	rBV3	25335	34566	2.06%	0.382%
30	20.326	2948	2951	2955	rVB	26719	34025	2.03%	0.376%
31	21.249	3104	3108	3114	rBV4	59307	93402	5.57%	1.033%
32	21.578	3156	3164	3168	rBV3	344445	642423	38.30%	7.107%
33	24.709	3689	3697	3706	rVB	170032	455494	27.15%	5.039%

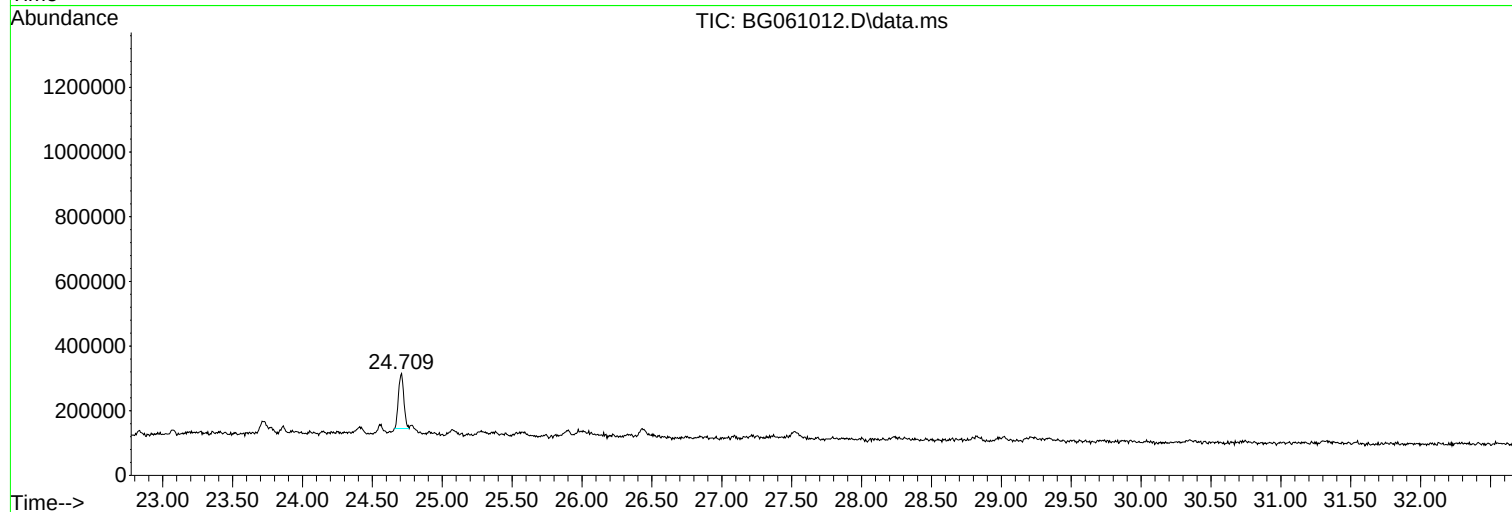
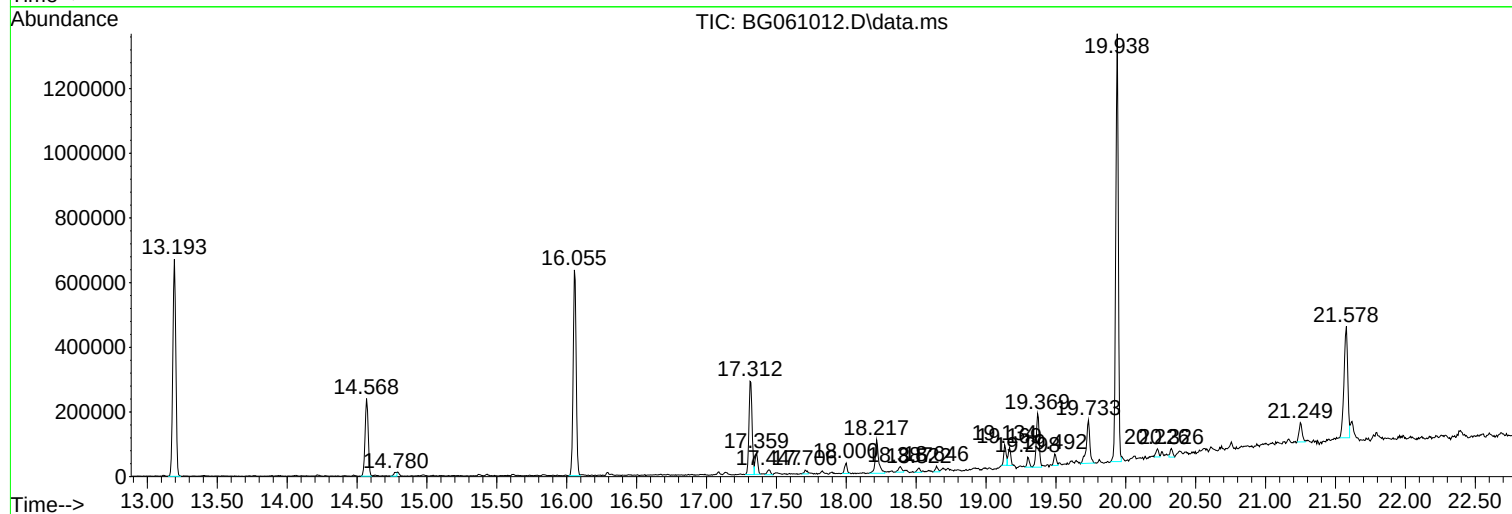
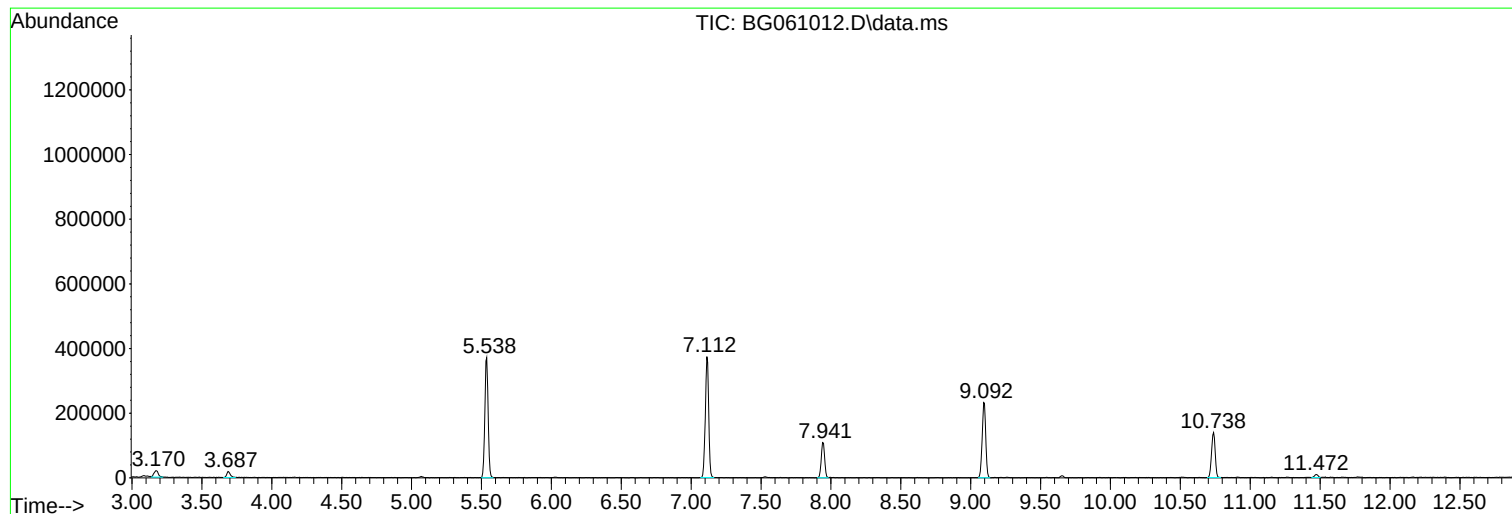
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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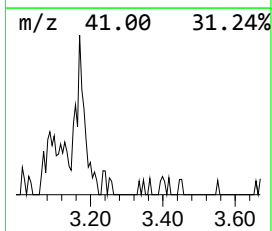
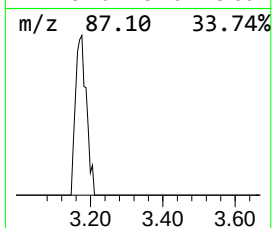
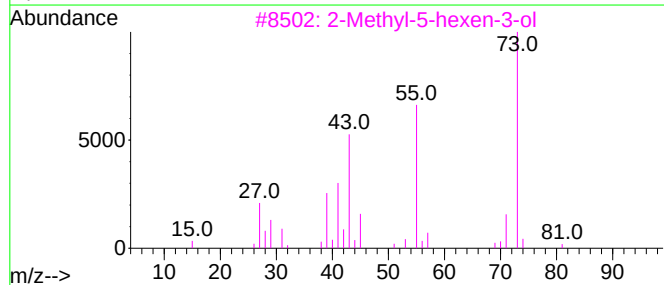
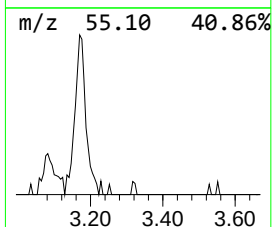
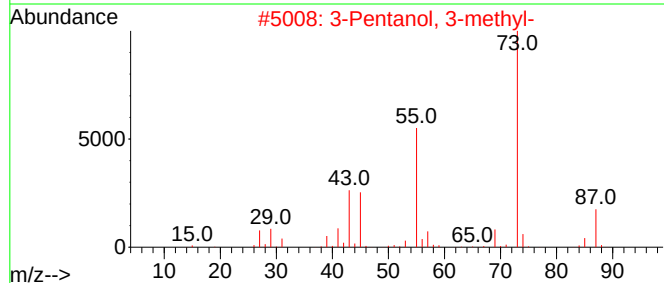
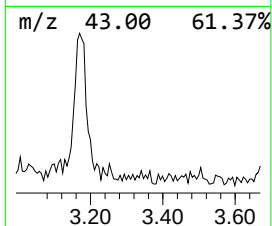
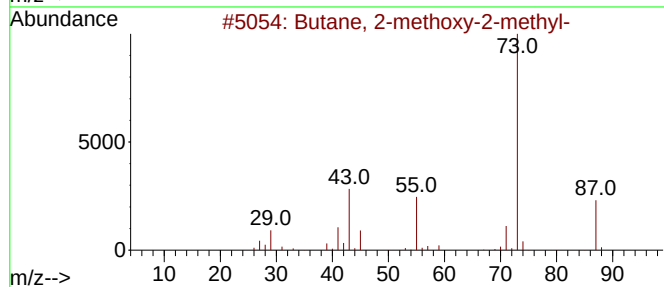
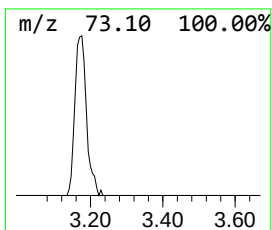
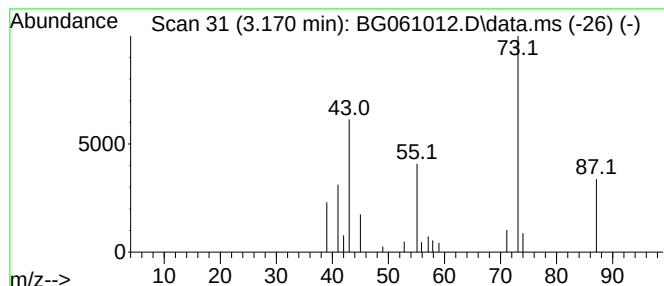
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.170	4.76 ng	43345	1,4-Dichlorobenzene-d4	7.947

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	45
3			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	12
4			1-Propene-1-thiol	74	C3H6S	000925-89-3	9
5			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9



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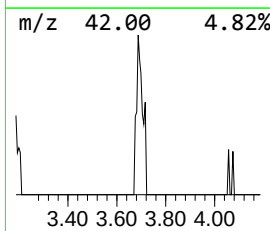
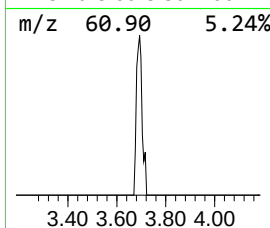
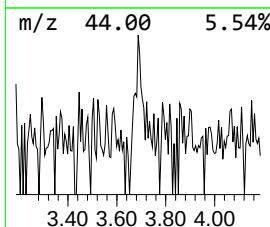
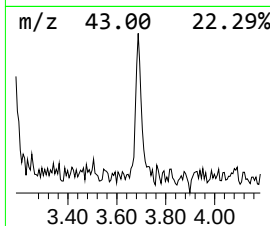
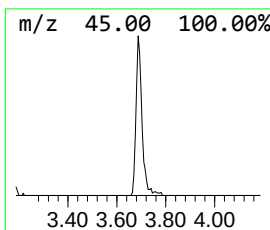
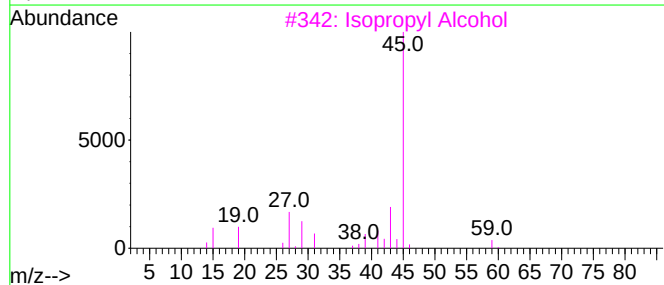
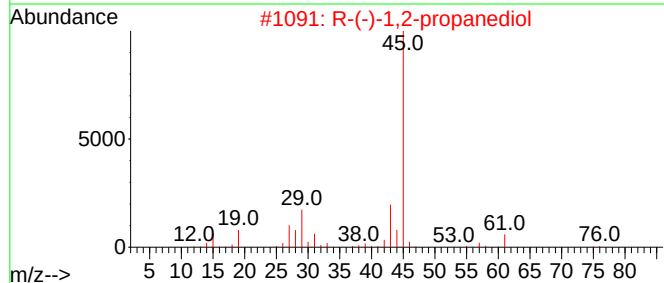
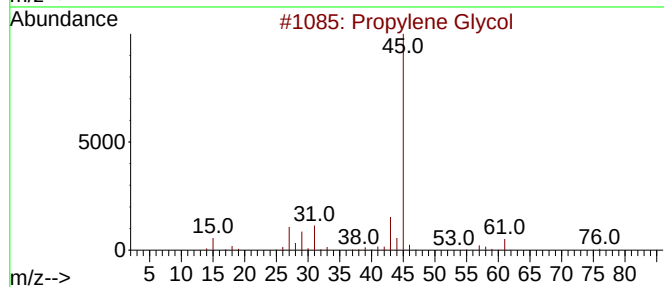
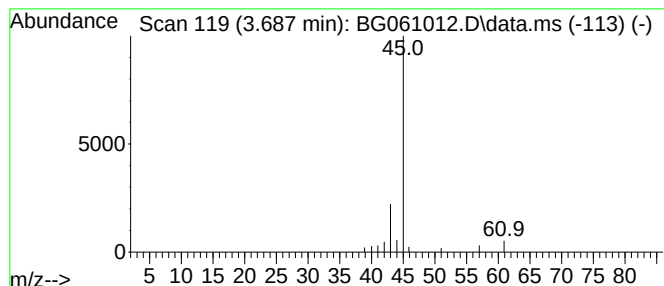
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown3.687 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.687	3.62 ng	32899	1,4-Dichlorobenzene-d4	7.947

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	9
2			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4			Formamide	45	CH3NO	000075-12-7	5
5			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	4



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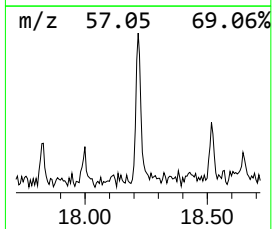
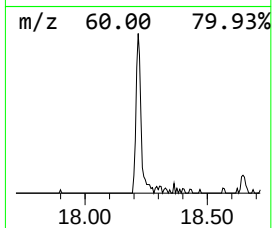
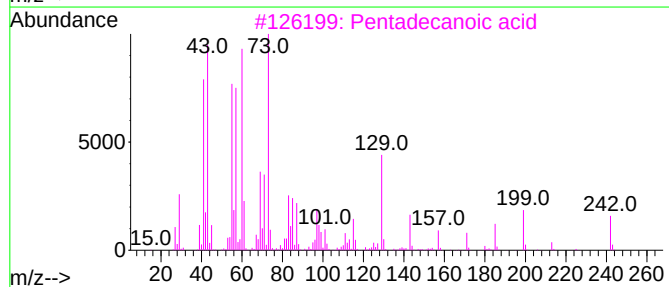
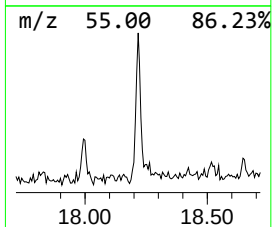
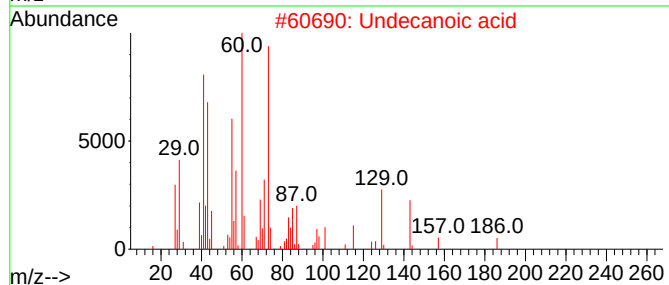
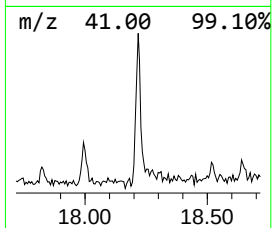
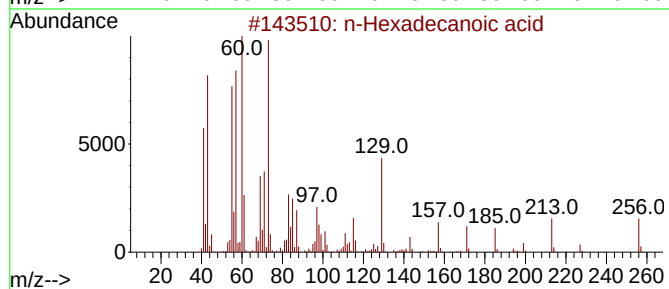
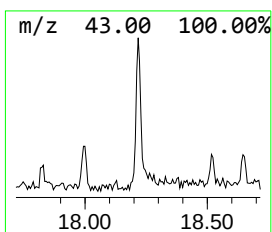
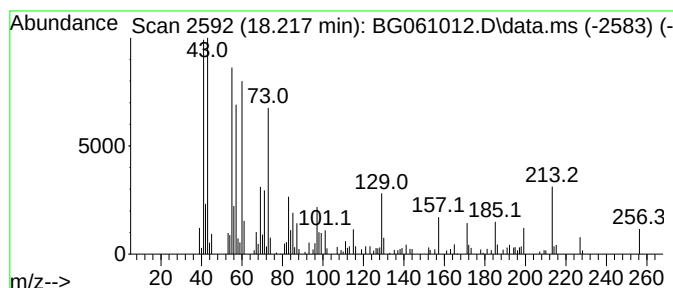
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.217	7.71 ng	177483	Phenanthrene-d10	17.318

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Undecanoic acid	186	C11H22O2	000112-37-8	83
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	62
4			Dodecanoic acid	200	C12H24O2	000143-07-7	52
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	52



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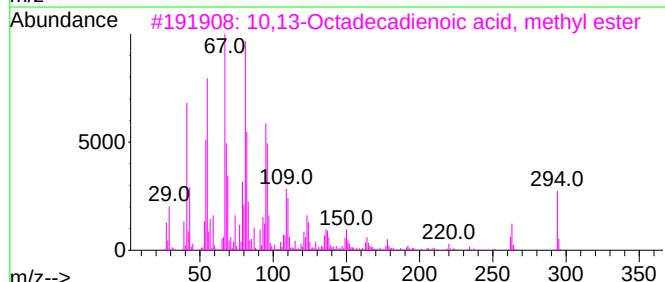
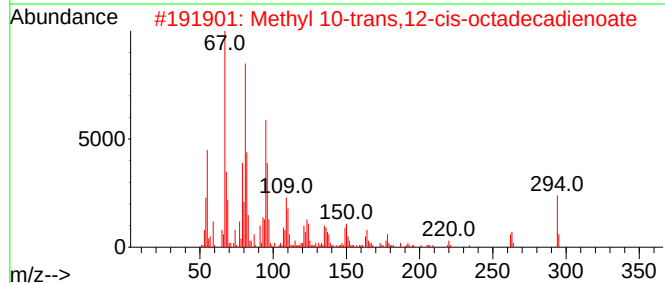
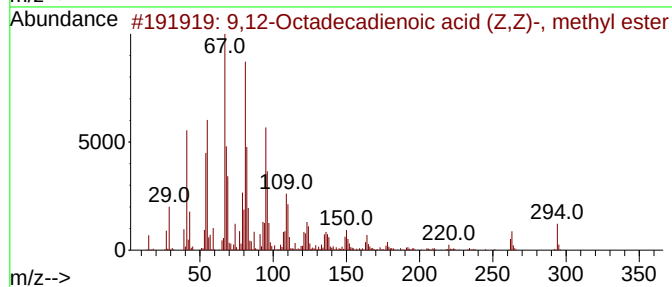
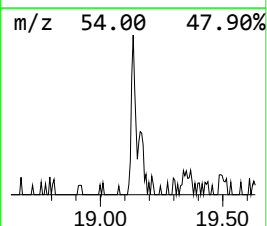
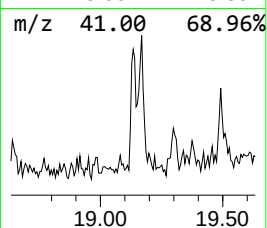
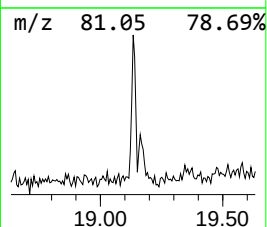
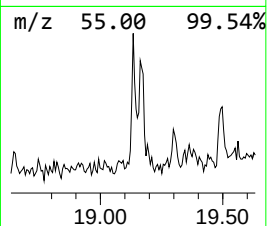
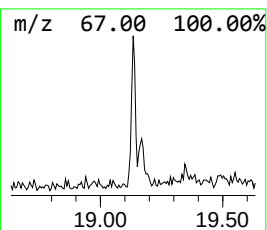
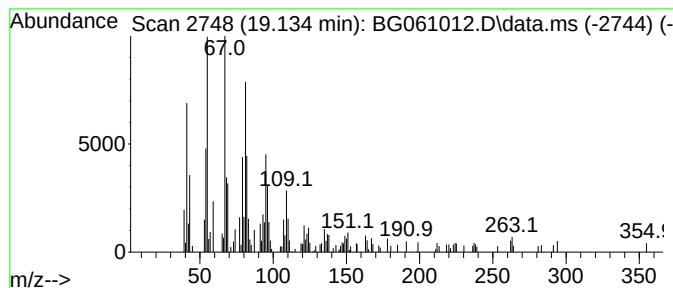
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9,12-Octadecadienoic acid (... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.134	3.36 ng	77419	Phenanthrene-d10	17.318

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	98
2			Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	97
3			10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	97
4			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	96
5			11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	94



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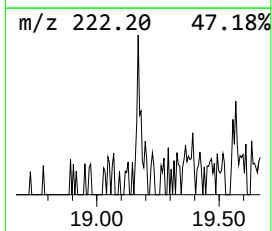
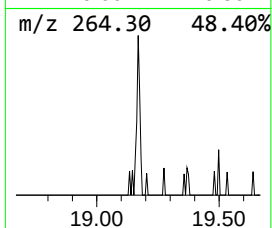
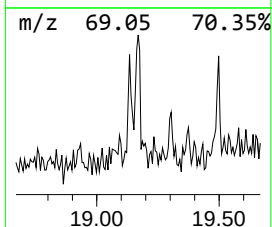
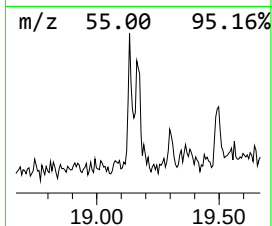
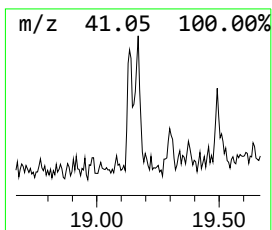
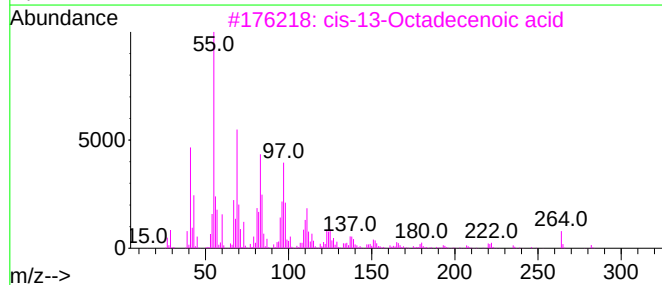
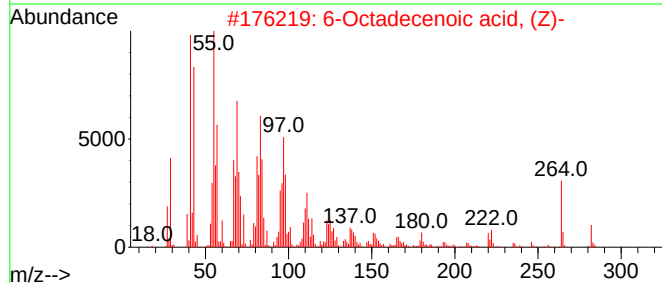
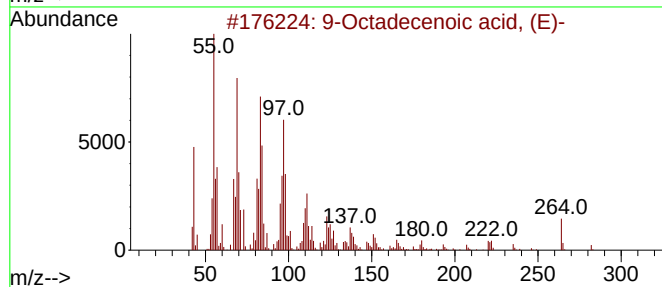
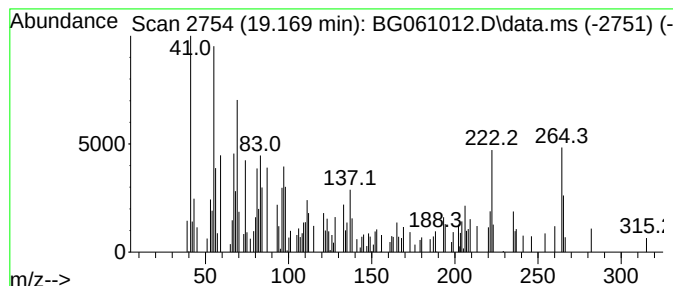
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 9-Octadecenoic acid, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.169	2.85 ng	65679	Phenanthrene-d10	17.318

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	93
2			6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	68
3			cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	55
4			12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	49
5			6-Octadecenoic acid	282	C18H34O2	1000336-66-8	49



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HD-02-04222024

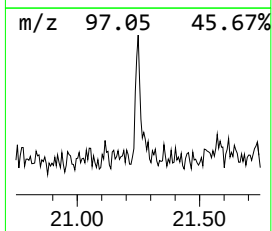
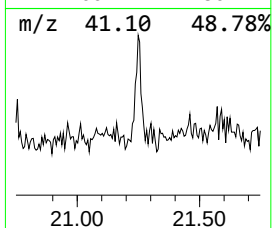
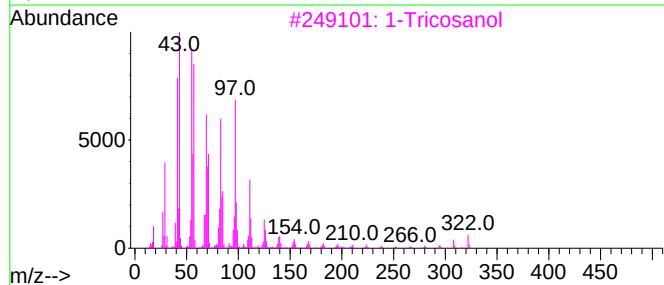
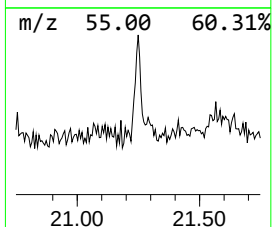
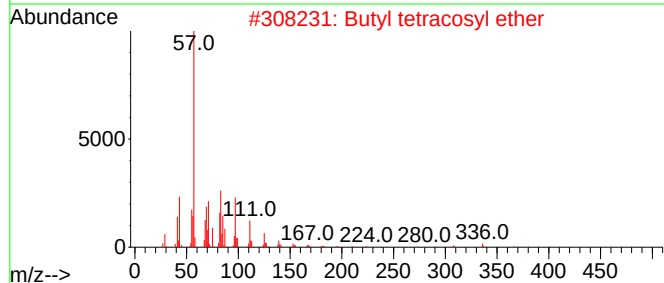
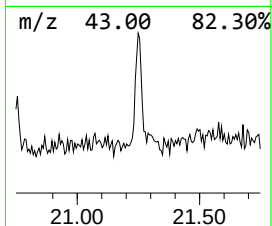
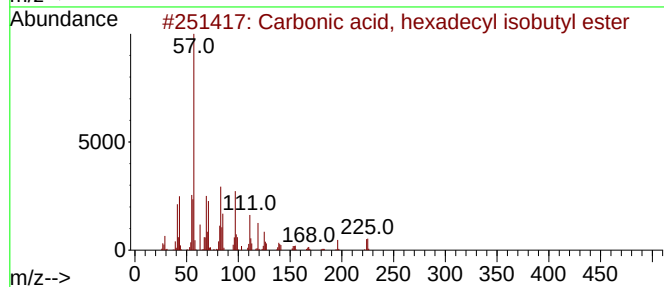
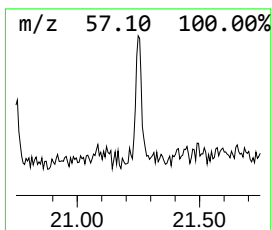
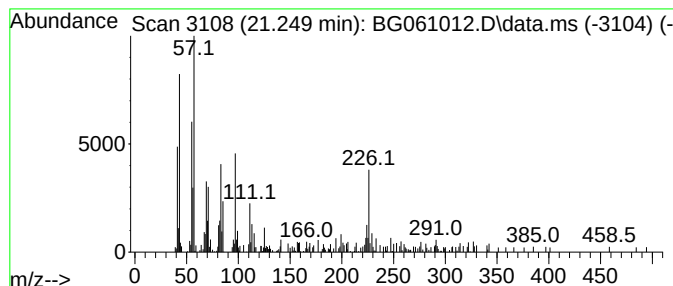
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Carbonic acid, hexadecyl is... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.249	2.91 ng	93402	Chrysene-d12	21.578

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, hexadecyl isobuty...	342	C21H42O3	1010314-61-3	58
2			Butyl tetracosyl ether	410	C28H58O	1000406-40-9	50
3			1-Tricosanol	340	C23H48O	003133-01-5	50
4			1-Tricosene	322	C23H46	018835-32-0	47
5			1-Octadecene	252	C18H36	000112-88-9	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042324\
Data File : BG061012.D
Acq On : 23 Apr 2024 17:57
Operator : MA/JU
Sample : P2227-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HD-02-04222024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042024.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...	3.170	4.8	ng	43345	1	7.947	181933	20.0
unknown3.687	3.687	3.6	ng	32899	1	7.947	181933	20.0
n-Hexadecanoic ...	18.217	7.7	ng	177483	4	17.318	460608	20.0
9,12-Octadecadi...	19.134	3.4	ng	77419	4	17.318	460608	20.0
9-Octadecenoic ...	19.169	2.9	ng	65679	4	17.318	460608	20.0
Carbonic acid, ...	21.249	2.9	ng	93402	5	21.578	642423	20.0