

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070121\
 Data File : BG049159.D
 Acq On : 1 Jul 2021 18:43
 Operator : CG/JU
 Sample : M2901-03
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 124033

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-BG063021.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049159.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.132	11	16	17	rBV2	33109	43831	1.51%	0.281%
2	3.220	27	31	38	rVB4	20617	44173	1.52%	0.283%
3	5.182	359	365	370	rBV	20378	35062	1.20%	0.225%
4	5.646	437	444	458	rBV	785854	1364937	46.90%	8.746%
5	7.245	708	716	729	rBV	840424	1507585	51.81%	9.660%
6	8.091	852	860	867	rBV	151443	260742	8.96%	1.671%
7	9.260	1050	1059	1067	rBV	530290	968703	33.29%	6.207%
8	10.670	1292	1299	1311	rBV	330309	577175	19.83%	3.698%
9	10.911	1330	1340	1348	rBV	194791	359069	12.34%	2.301%
10	13.355	1746	1756	1765	rBV	1273215	1987685	68.30%	12.737%
11	14.730	1984	1990	1998	rVB	305135	498607	17.13%	3.195%
12	16.222	2237	2244	2256	rBV	1177801	1813929	62.33%	11.623%
13	17.480	2452	2458	2463	rBV	379773	586304	20.15%	3.757%
14	17.521	2463	2465	2471	rVB	37513	50257	1.73%	0.322%
15	18.138	2566	2570	2575	rBV2	51968	73617	2.53%	0.472%
16	18.361	2603	2608	2613	rBV2	87473	127591	4.38%	0.818%
17	19.307	2765	2769	2774	rVB2	90790	114587	3.94%	0.734%
18	19.530	2802	2807	2812	rVB	69424	99861	3.43%	0.640%
19	19.630	2820	2824	2828	rBV5	29332	38693	1.33%	0.248%
20	19.894	2865	2869	2877	rVB	66044	126966	4.36%	0.814%
21	20.088	2896	2902	2908	rBV	2167151	2910090	100.00%	18.647%
22	20.376	2944	2951	2957	rVB9	14639	36710	1.26%	0.235%
23	21.399	3120	3125	3134	rBV5	77383	157089	5.40%	1.007%
24	21.651	3162	3168	3174	rVB	311129	459070	15.78%	2.942%
25	21.769	3180	3188	3193	rBV	377360	680297	23.38%	4.359%
26	24.019	3565	3571	3577	rBV3	25524	71461	2.46%	0.458%
27	25.077	3742	3751	3762	rBV2	212720	611940	21.03%	3.921%

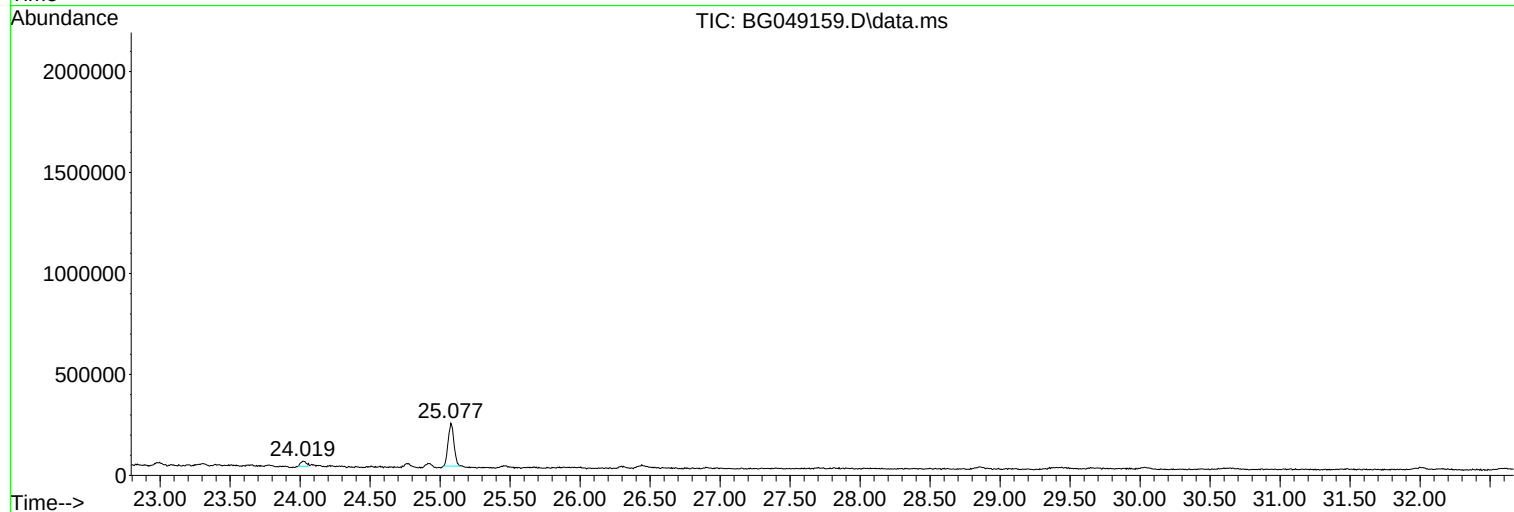
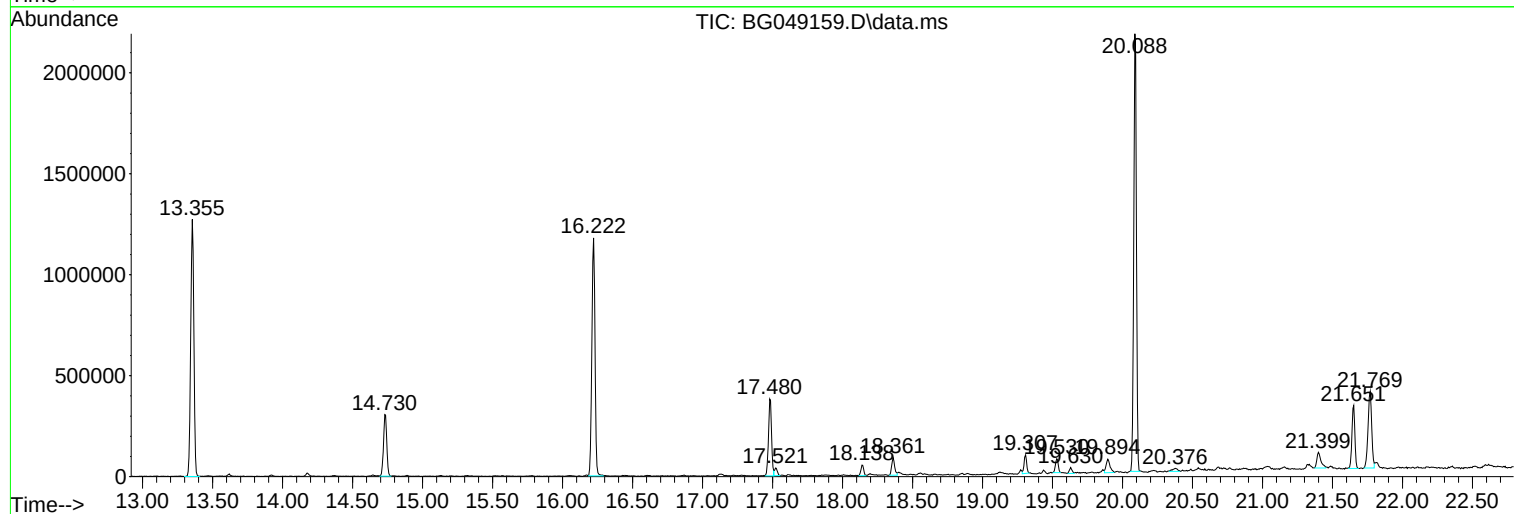
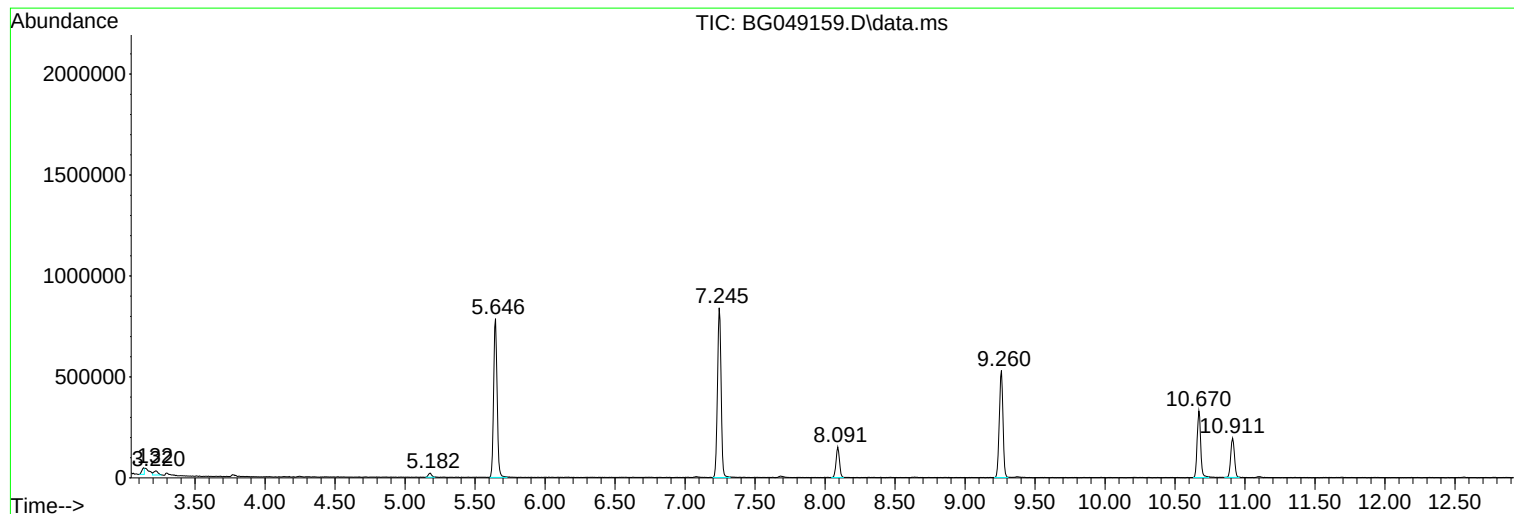
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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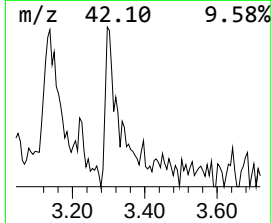
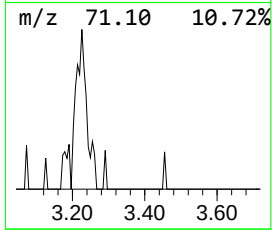
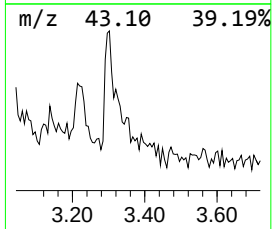
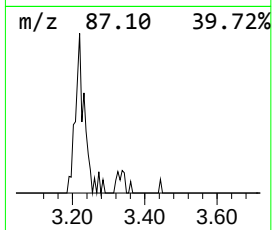
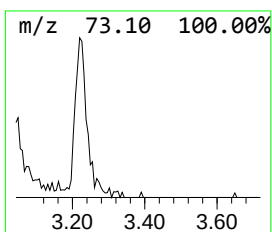
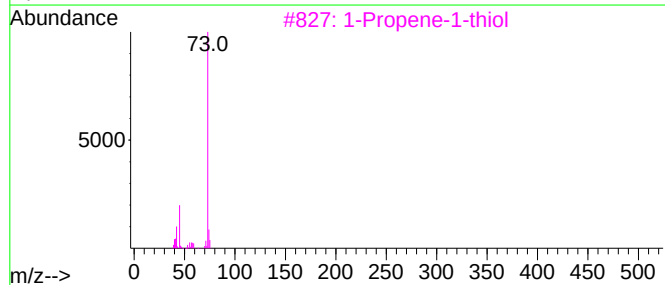
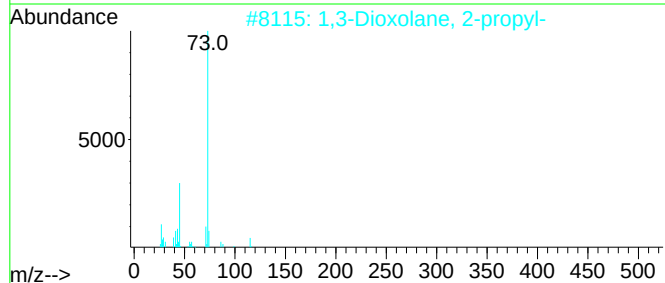
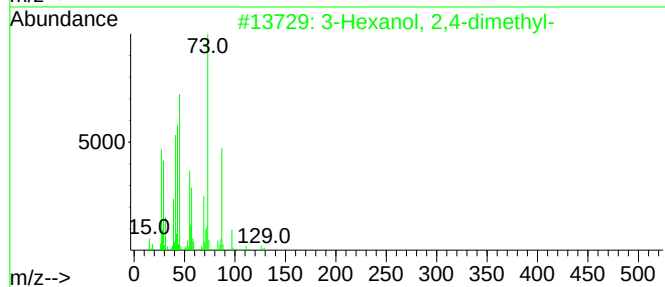
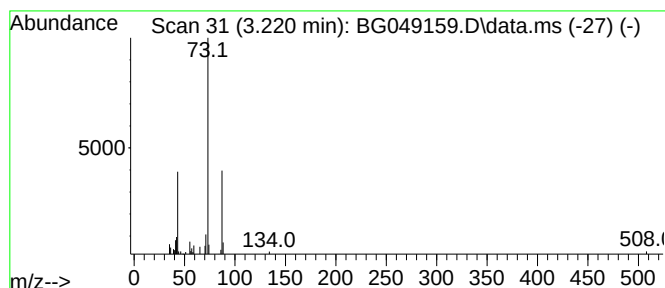
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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Peak Number 2 unknown3.220 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.220	3.39 ng	44173	1,4-Dichlorobenzene-d4	8.091

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	40
2		1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	10
3		1-Propene-1-thiol	74	C3H6S	000925-89-3	9
4		3-Dodecanol, 3,7,11-trimethyl-	228	C15H32O	007278-65-1	9
5		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	9



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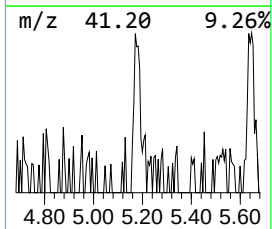
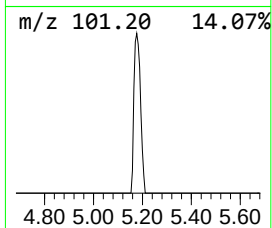
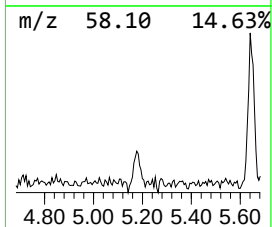
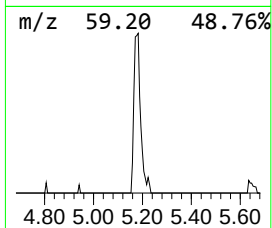
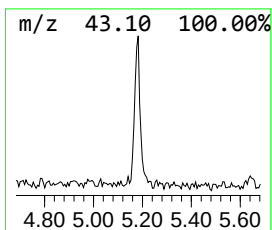
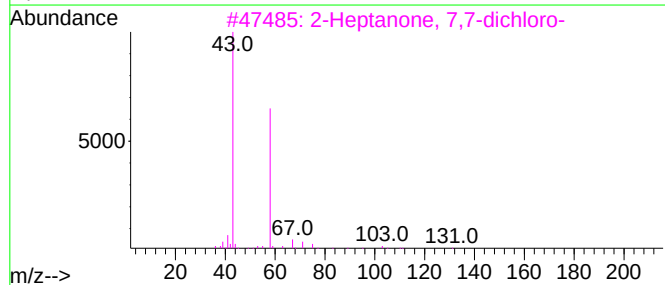
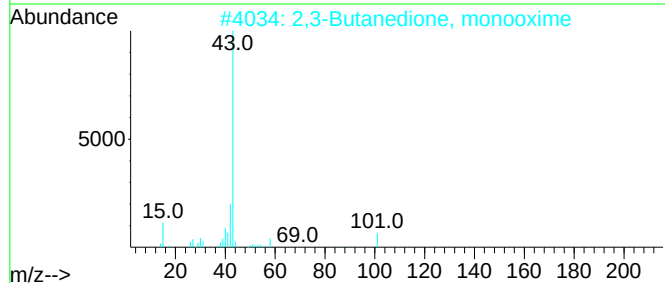
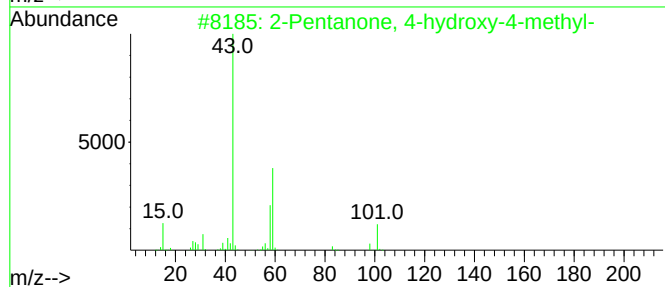
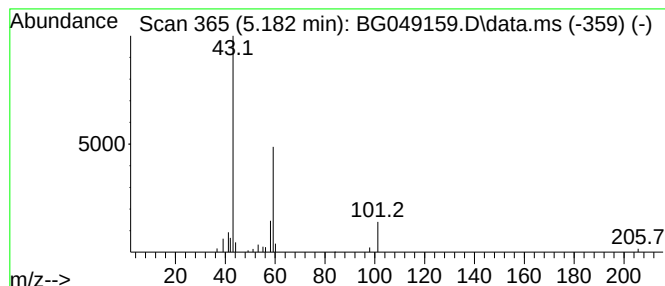
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.182	2.69 ng	35062	1,4-Dichlorobenzene-d4	8.091

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
3	2-Heptanone, 7,7-dichloro-	182	C7H12Cl2O	066241-43-8	9		
4	tert-Butyl Hydroperoxide	90	C4H10O2	000075-91-2	9		
5	Tetramethylammonium acetate	133	C6H15NO2	010581-12-1	9		



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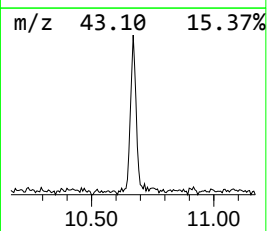
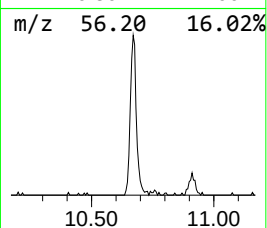
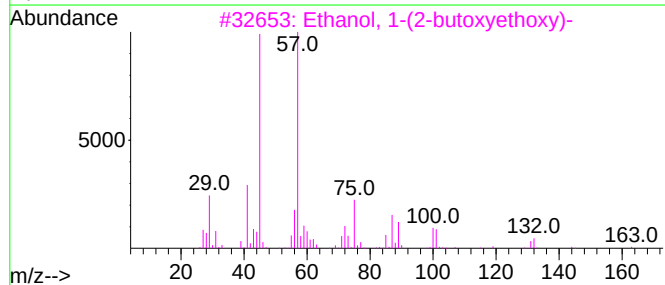
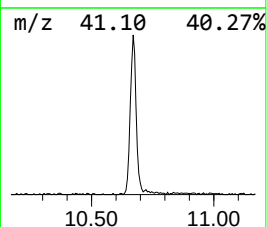
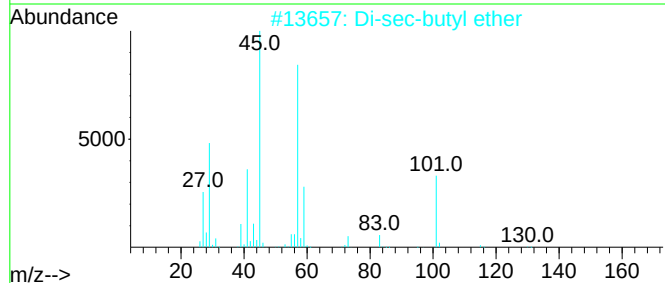
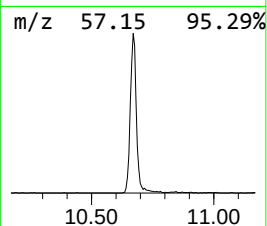
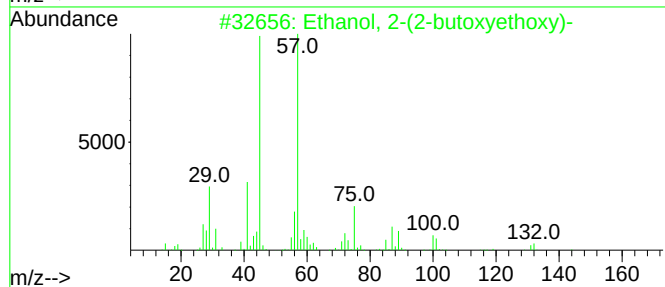
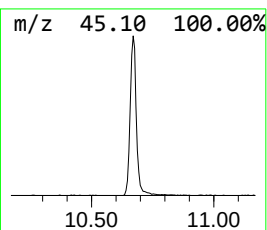
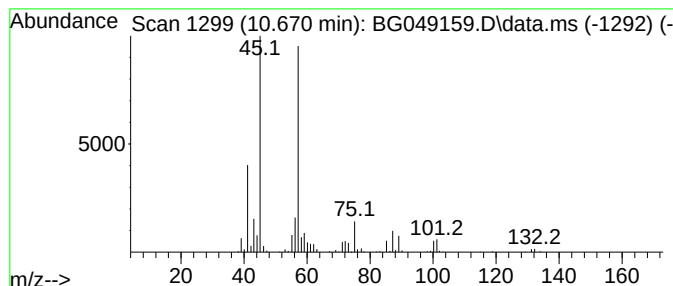
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Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.670	32.15 ng	577175	Naphthalene-d8	10.911

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2			Di-sec-butyl ether	130	C8H18O	006863-58-7	53
3			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
4			Propanoic acid, 2-hydroxy-, buty...	146	C7H14O3	000138-22-7	50
5			Hexaethylene glycol	282	C12H26O7	002615-15-8	50



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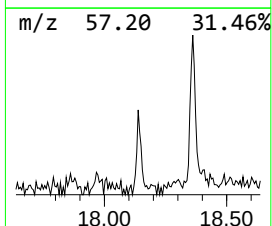
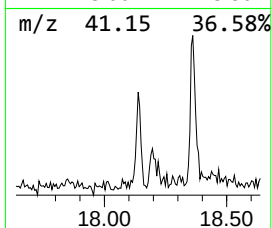
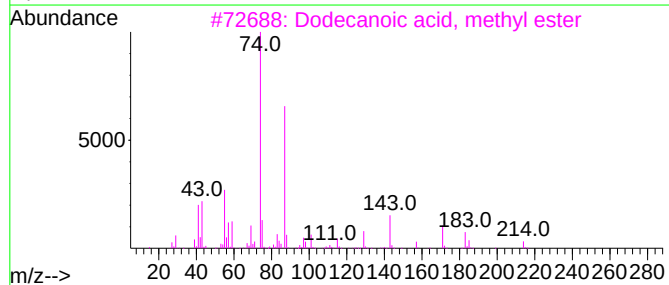
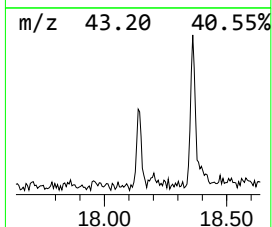
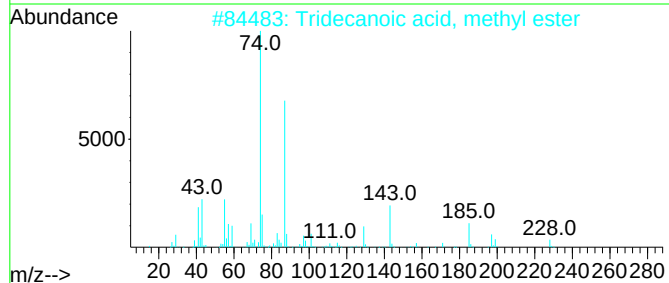
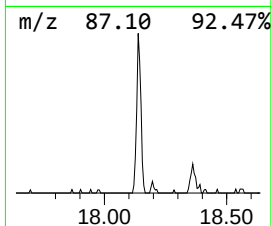
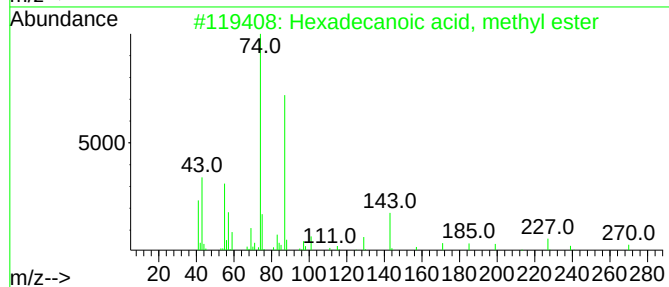
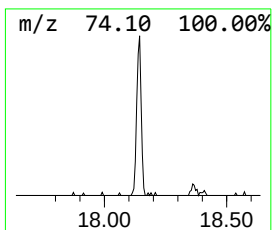
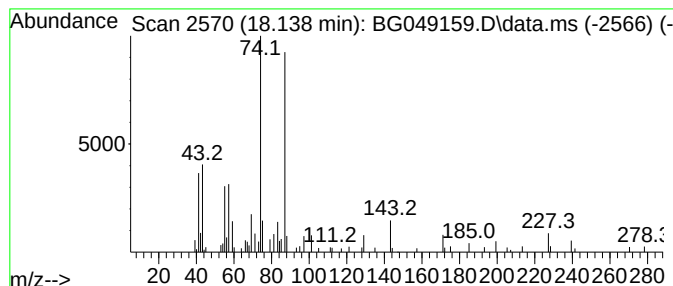
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Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.138	2.51 ng	73617	Phenanthrene-d10	17.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	94
2			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	86
3			Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	78
4			Methyl tetradecanoate	242	C15H30O2	000124-10-7	72
5			Methyl 8-methyl-nonanoate	186	C11H22O2	1000336-43-6	64



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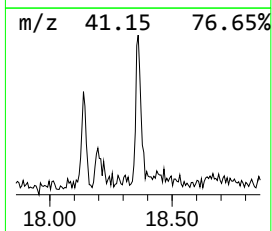
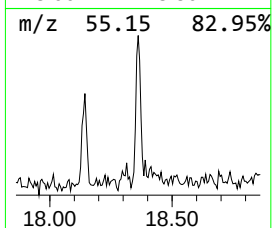
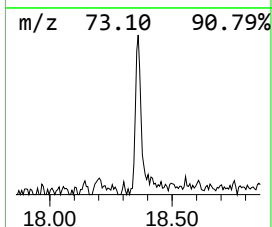
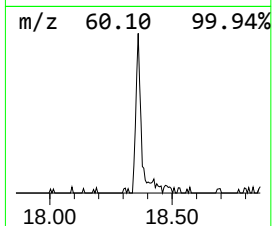
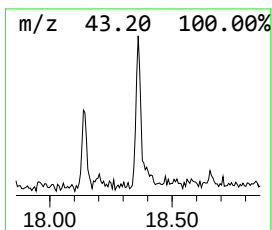
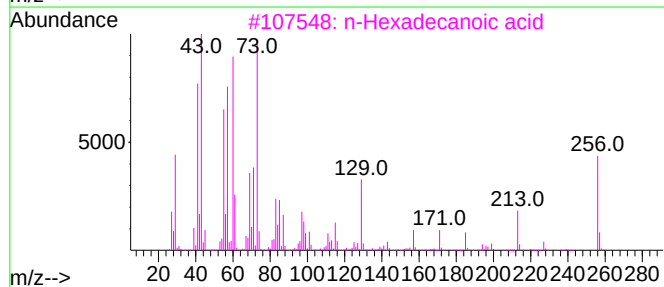
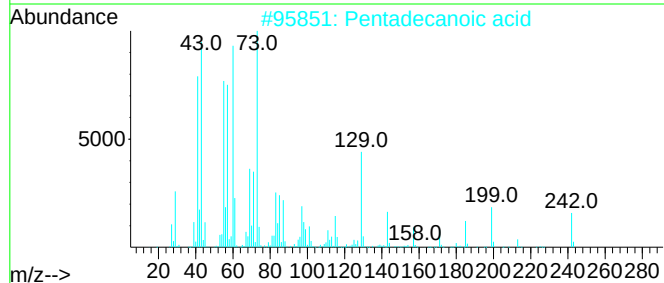
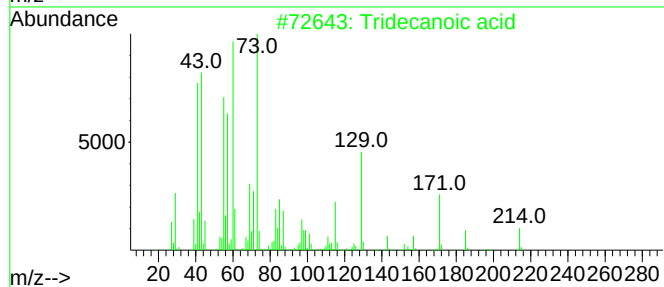
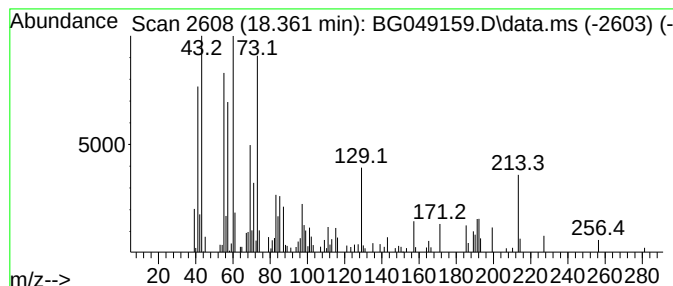
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Peak Number 6 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.361	4.35 ng	127591	Phenanthrene-d10	17.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	81
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Undecanoic acid	186	C11H22O2	000112-37-8	60



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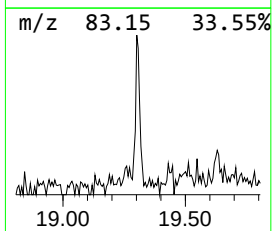
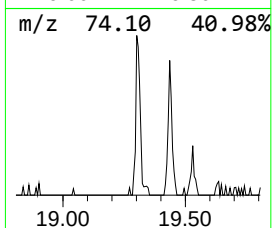
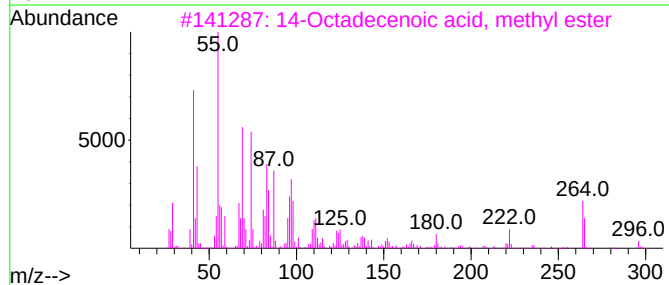
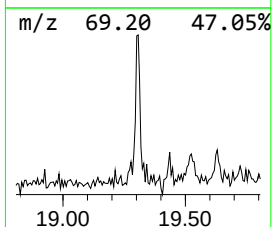
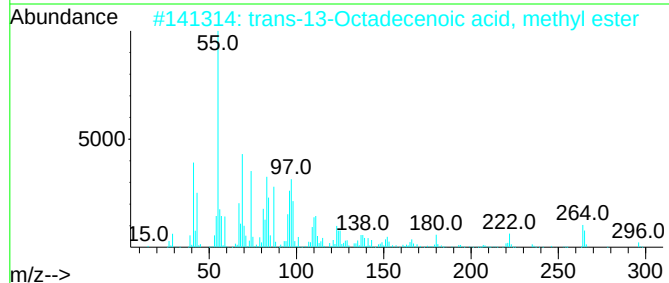
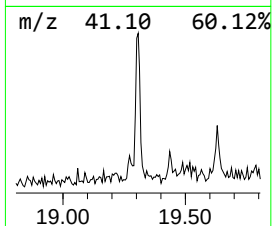
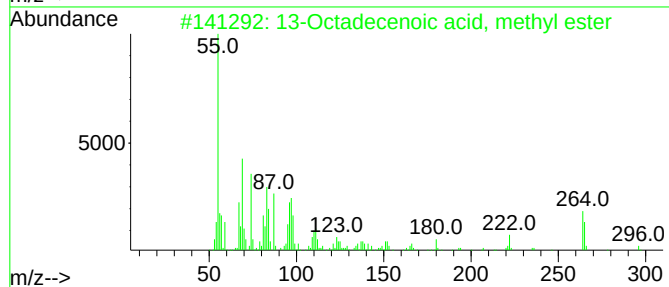
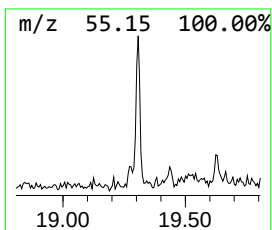
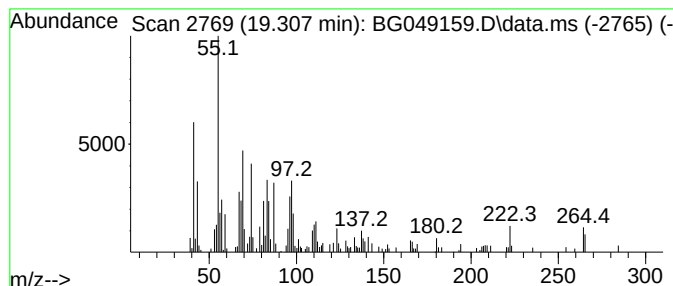
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 13-Octadecenoic acid, methy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.307	3.91 ng	114587	Phenanthrene-d10	17.480

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	90
2		trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	87
3		14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	83
4		10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	74
5		Cyclopropanoic acid, 2-hex...	282	C18H34O2	010152-61-1	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070121\
Data File : BG049159.D
Acq On : 1 Jul 2021 18:43
Operator : CG/JU
Sample : M2901-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
124033

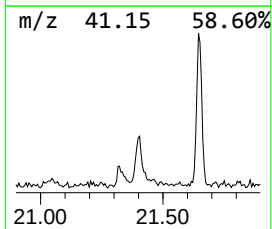
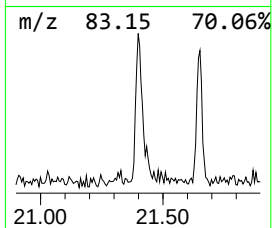
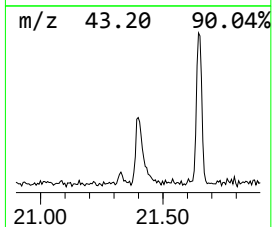
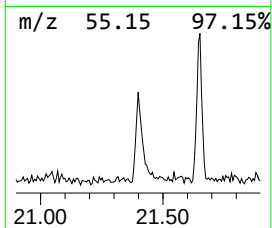
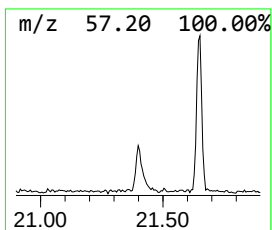
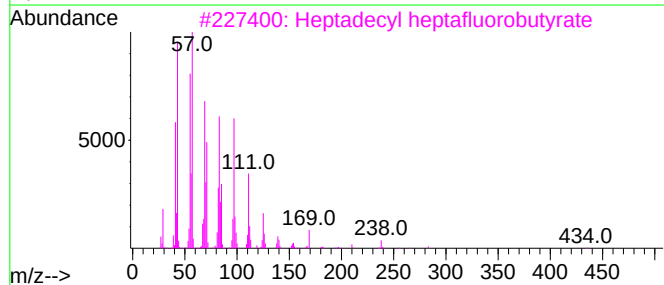
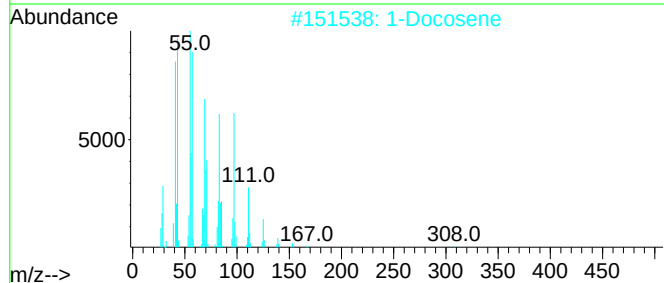
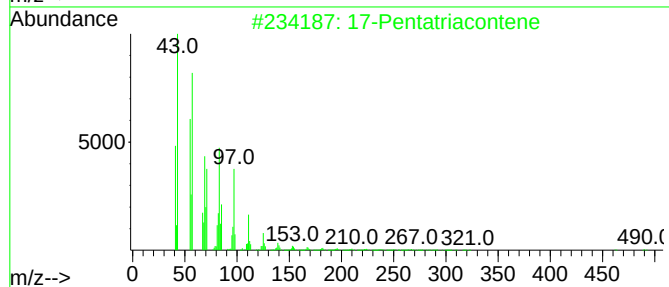
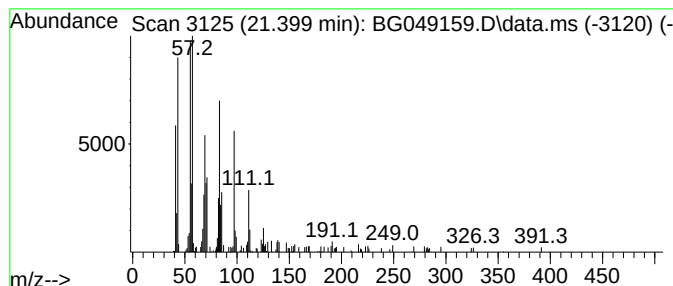
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 17-Pentatriacontene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.399	4.62 ng	157089	Chrysene-d12	21.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene			491	C35H70	006971-40-0	91
2	1-Docosene			308	C22H44	001599-67-3	90
3	Heptadecyl heptafluorobutyrate			452	C21H35F7O2	959085-66-6	90
4	1-Heptadecene			238	C17H34	006765-39-5	89
5	Carbonic acid, hexadecyl 2,2,2-t...			416	C19H35Cl3O3	1000314-56-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070121\
Data File : BG049159.D
Acq On : 1 Jul 2021 18:43
Operator : CG/JU
Sample : M2901-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
124033

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.220	3.220	3.4	ng	44173	1	8.091	260742	20.0
2-Pentanone, 4-...	5.182	2.7	ng	35062	1	8.091	260742	20.0
Ethanol, 2-(2-b...	10.670	32.1	ng	577175	2	10.911	359069	20.0
Hexadecanoic ac...	18.138	2.5	ng	73617	4	17.480	586304	20.0
Tridecanoic acid	18.361	4.3	ng	127591	4	17.480	586304	20.0
13-Octadecenoic...	19.307	3.9	ng	114587	4	17.480	586304	20.0
17-Pentatriacon...	21.399	4.6	ng	157089	5	21.769	680297	20.0