

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
 Data File : BG048982.D
 Acq On : 15 Jun 2021 18:00
 Operator : CG/JU
 Sample : M2672-05
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 17-B6(24-28)

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-BG061121.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048982.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.160	16	21	31	rVB	116338	206653	9.47%	1.888%
2	3.284	38	42	51	rVB2	43100	67992	3.11%	0.621%
3	5.199	362	368	374	rVB	17702	31749	1.45%	0.290%
4	5.669	440	448	456	rBV	568496	964933	44.20%	8.814%
5	5.734	456	459	467	rVB	14191	29008	1.33%	0.265%
6	7.267	712	720	731	rBV	562624	1020983	46.76%	9.326%
7	8.113	857	864	871	rBV	121302	216097	9.90%	1.974%
8	9.283	1053	1063	1071	rBV	346874	633248	29.00%	5.784%
9	10.699	1299	1304	1310	rBV2	12135	23379	1.07%	0.214%
10	10.939	1338	1345	1353	rVB	153734	286062	13.10%	2.613%
11	13.378	1750	1760	1769	rBV	794496	1286473	58.92%	11.751%
12	14.758	1987	1995	2002	rBV	246648	400623	18.35%	3.659%
13	16.157	2224	2233	2238	rBV2	28875	42519	1.95%	0.388%
14	16.245	2241	2248	2259	rVV	793063	1215655	55.68%	11.104%
15	17.508	2456	2463	2470	rVB	343176	537546	24.62%	4.910%
16	17.626	2476	2483	2487	rVB5	21161	30154	1.38%	0.275%
17	18.389	2608	2613	2620	rBV2	64409	97478	4.46%	0.890%
18	19.312	2767	2770	2776	rBV6	11256	21953	1.01%	0.201%
19	19.653	2820	2828	2834	rBV5	56495	87117	3.99%	0.796%
20	20.111	2900	2906	2912	rBV	1597204	2183248	100.00%	19.942%
21	20.869	3031	3035	3039	rBV6	16726	23503	1.08%	0.215%
22	21.433	3127	3131	3136	rBV4	33855	56223	2.58%	0.514%
23	21.686	3170	3174	3179	rVB2	32111	49167	2.25%	0.449%
24	21.797	3187	3193	3202	rVB	399109	674997	30.92%	6.166%
25	22.003	3225	3228	3234	rVB4	15689	23496	1.08%	0.215%
26	22.637	3332	3336	3342	rBV7	12676	23751	1.09%	0.217%
27	23.019	3397	3401	3412	rVB7	21548	42808	1.96%	0.391%
28	25.129	3750	3760	3771	rBV2	216043	671092	30.74%	6.130%

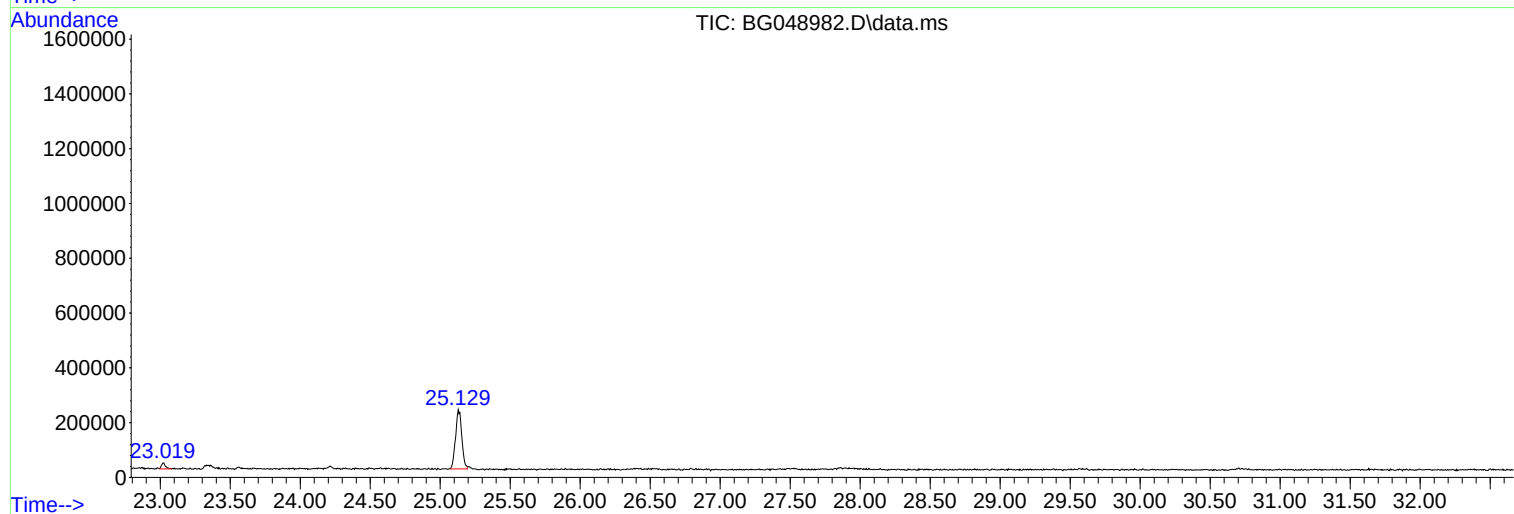
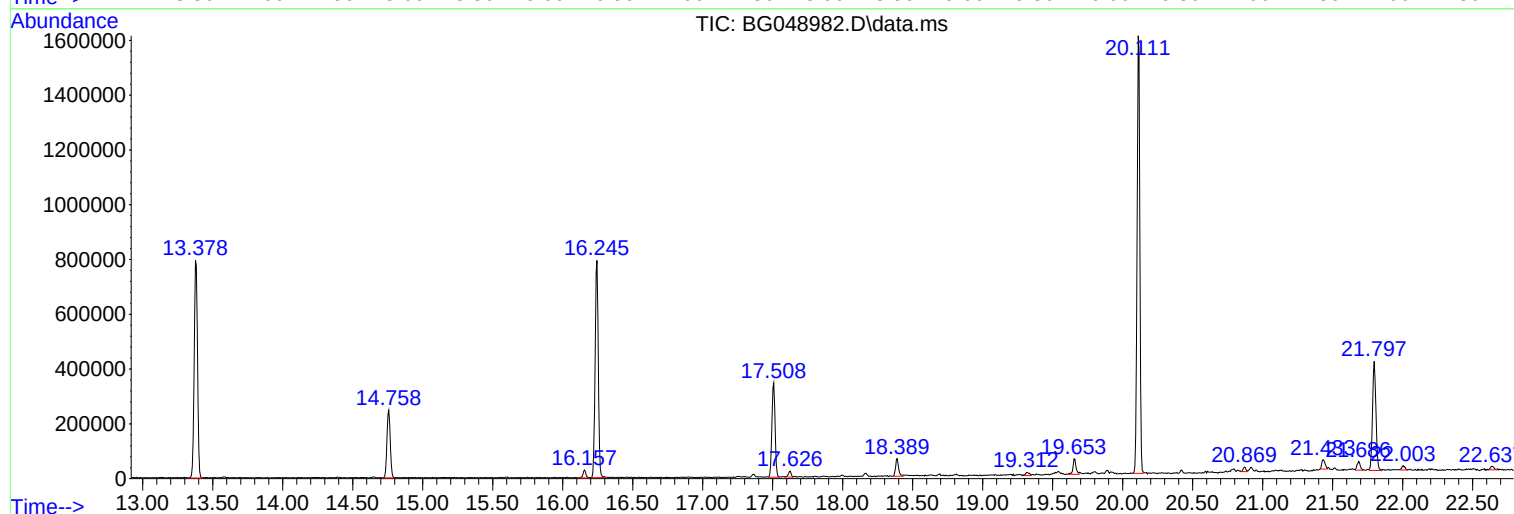
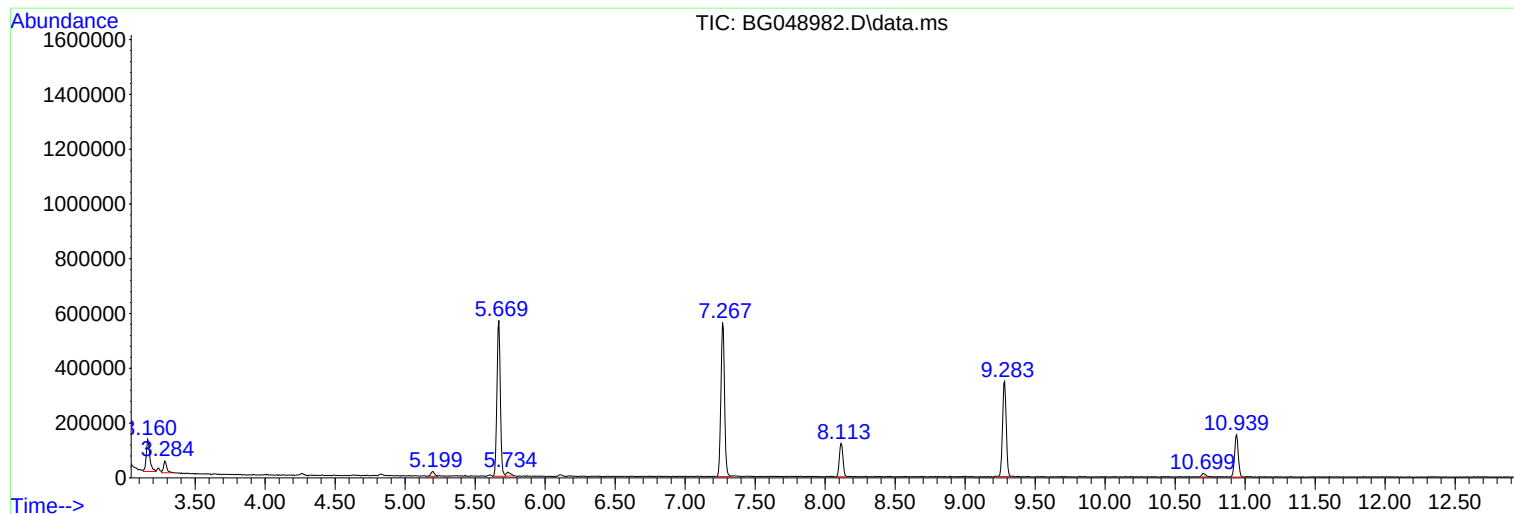
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Instrument :
BNA_G
ClientSampleId :
17-B6(24-28)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.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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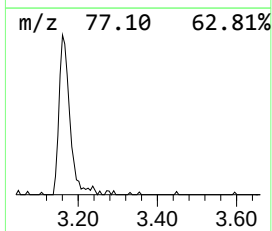
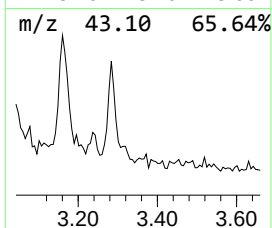
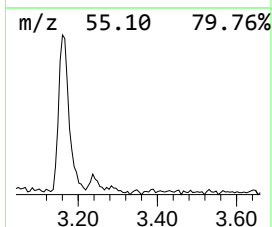
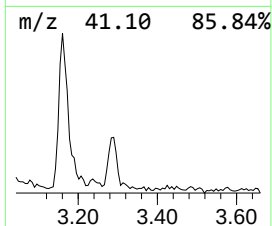
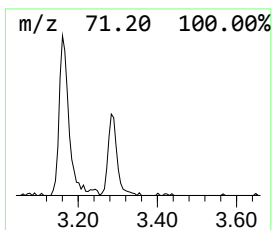
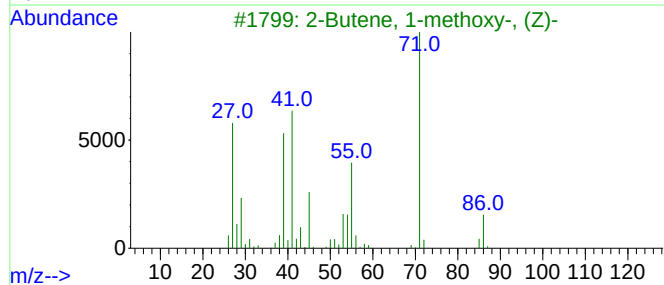
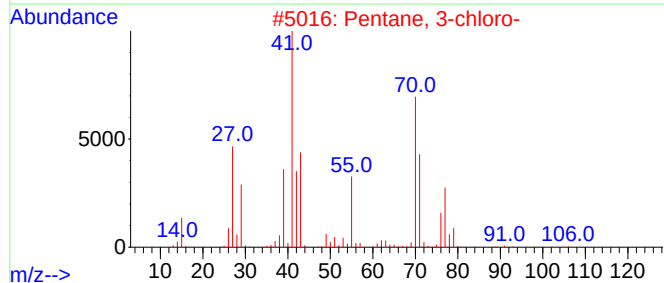
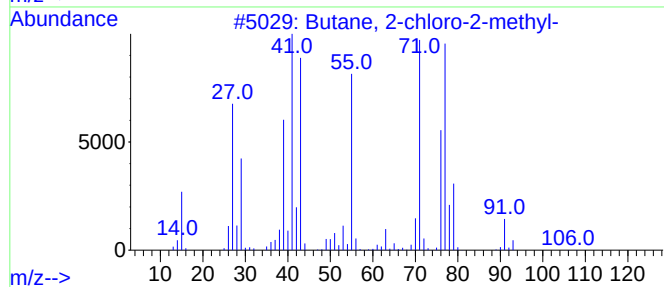
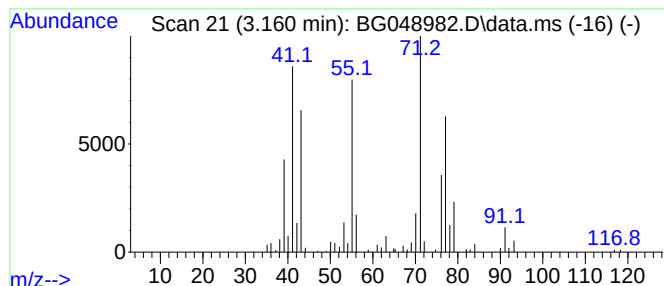
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.160	19.13 ng	206653	1,4-Dichlorobenzene-d4	8.113

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-chloro-2-methyl-	106	C5H11Cl	000594-36-5	78
2			Pentane, 3-chloro-	106	C5H11Cl	000616-20-6	50
3			2-Butene, 1-methoxy-, (Z)-	86	C5H10O	010034-16-9	32
4			2-Penten-1-ol, 2-methyl-, (E)-	100	C6H12O	016958-19-3	25
5			1-Hexene, 4,5-dimethyl-	112	C8H16	016106-59-5	23



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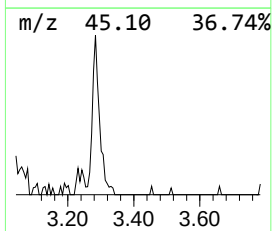
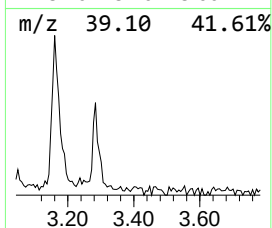
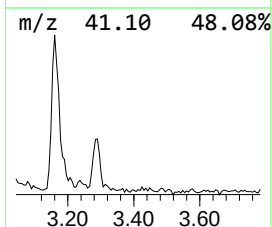
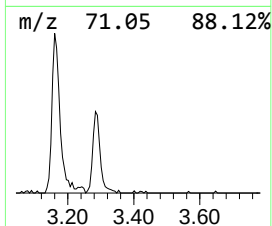
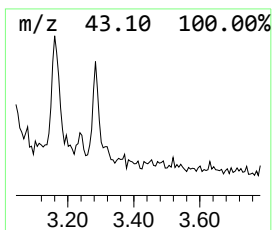
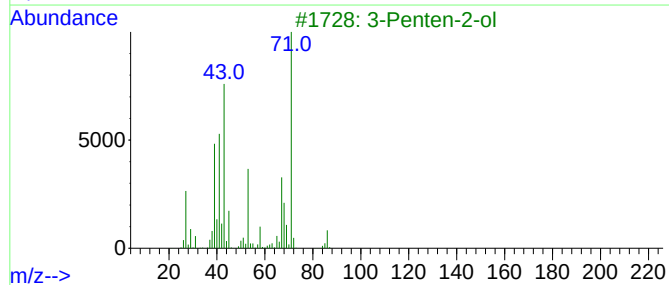
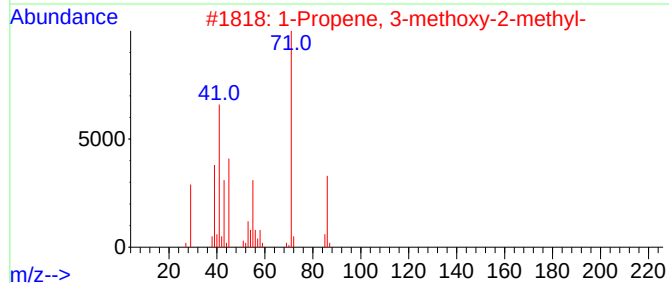
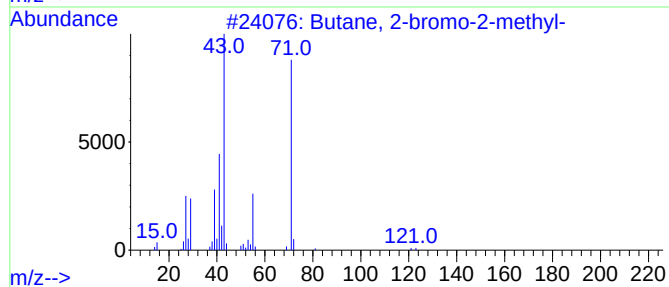
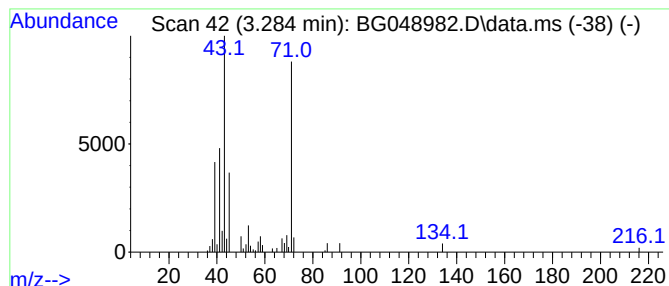
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown3.284 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.284	6.29 ng	67992	1,4-Dichlorobenzene-d4	8.113

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-bromo-2-methyl-	150	C5H11Br	000507-36-8	47
2			1-Propene, 3-methoxy-2-methyl-	86	C5H10O	022418-49-1	47
3			3-Penten-2-ol	86	C5H10O	001569-50-2	45
4			4,4-Dimethyl-1-hexene	112	C8H16	001647-08-1	43
5			3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	43



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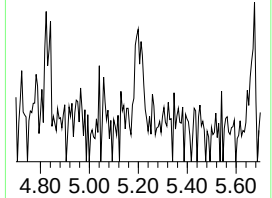
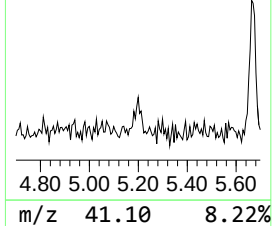
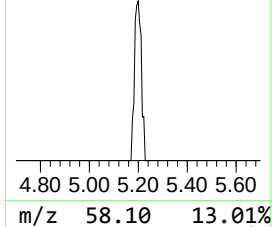
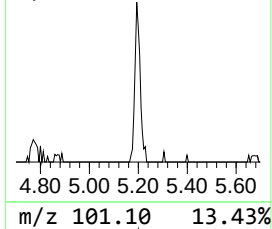
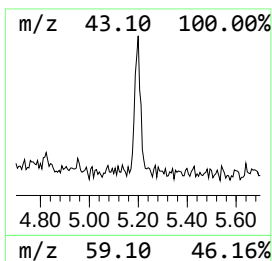
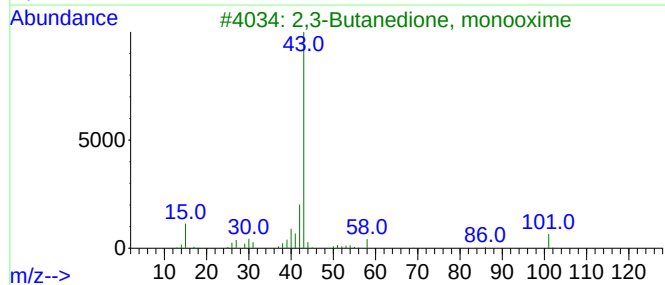
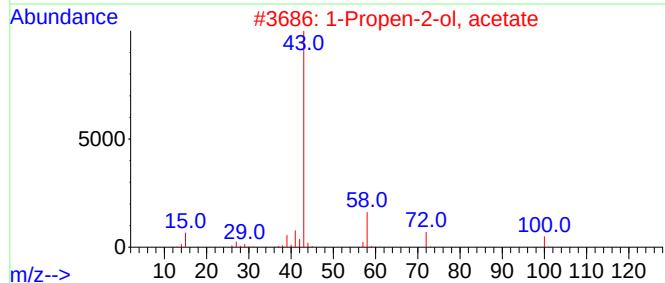
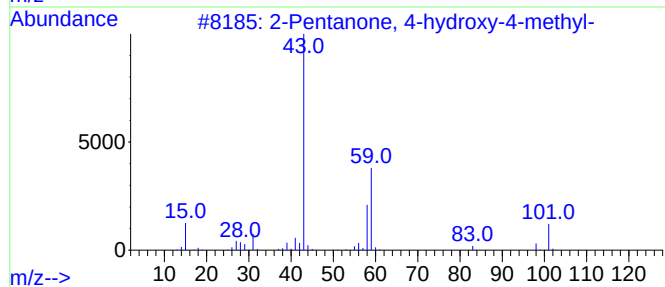
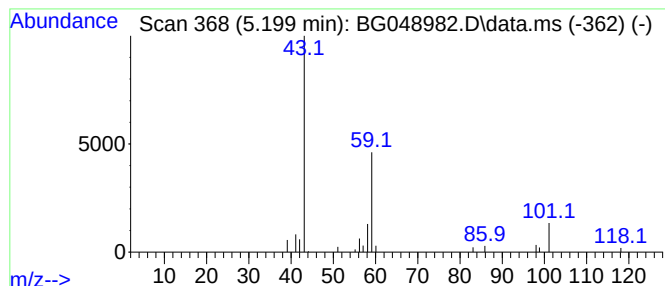
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.199	2.94 ng	31749	1,4-Dichlorobenzene-d4	8.113

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	7
4		Diacetamide	101	C4H7NO2	000625-77-4	7
5		Butane	58	C4H10	000106-97-8	5



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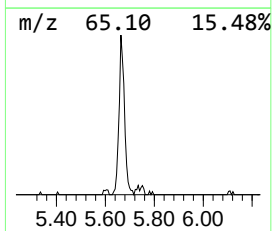
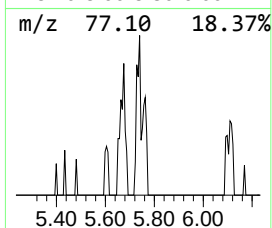
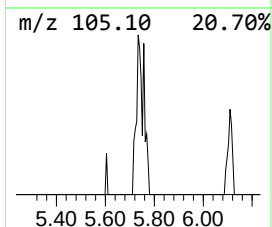
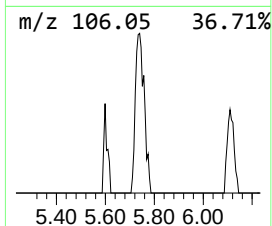
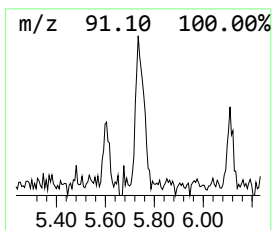
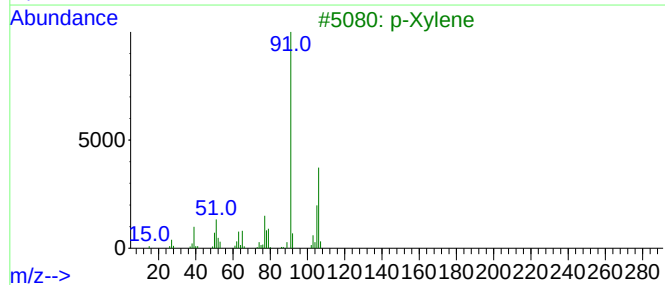
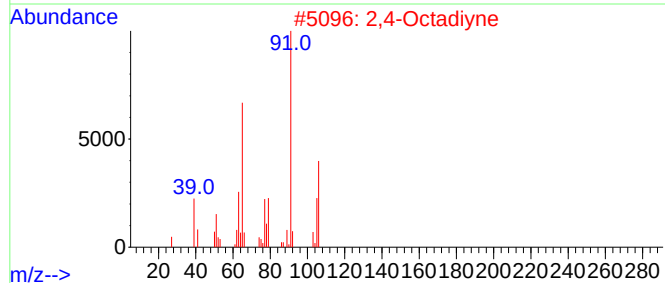
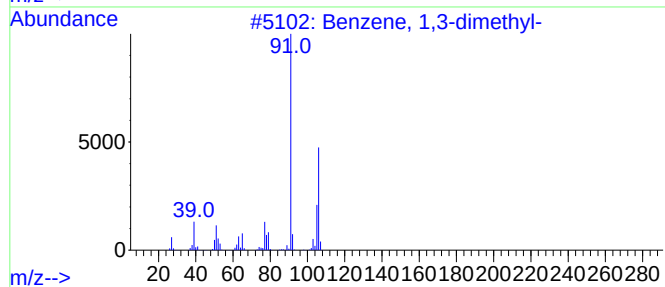
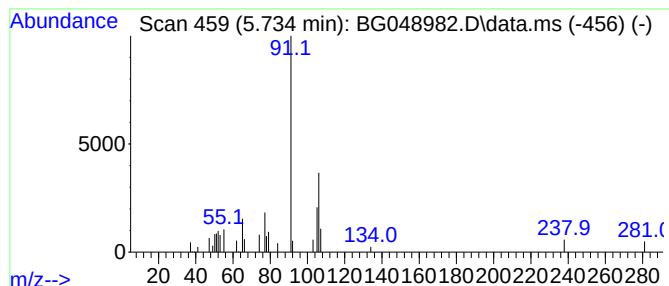
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Peak Number 4 Benzene, 1,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.734	2.68 ng	29008	1,4-Dichlorobenzene-d4	8.113

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	58
2			2,4-Octadiyne	106	C8H10	002809-71-4	52
3			p-Xylene	106	C8H10	000106-42-3	50
4			1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	49
5			o-Xylene	106	C8H10	000095-47-6	47



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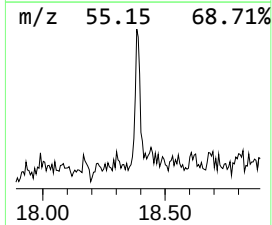
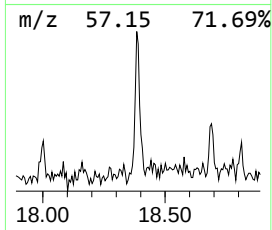
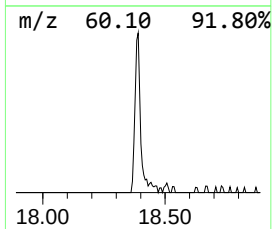
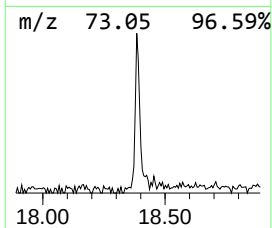
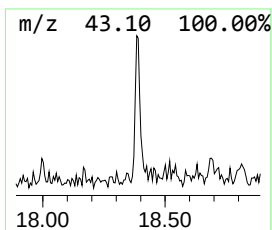
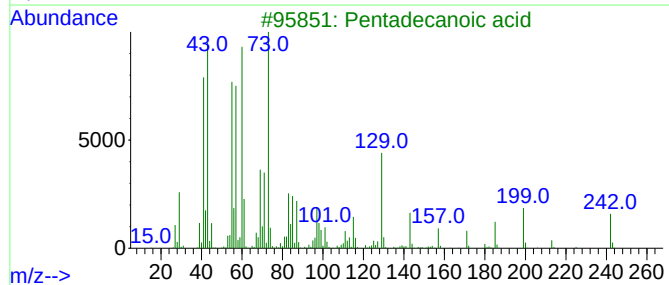
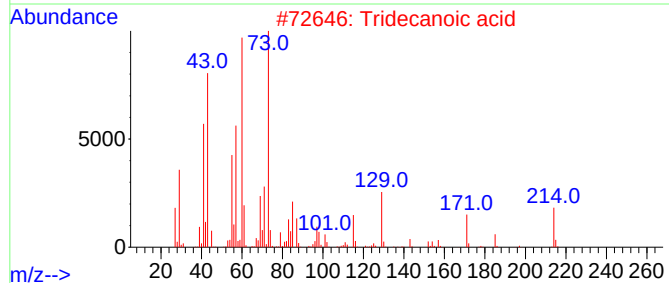
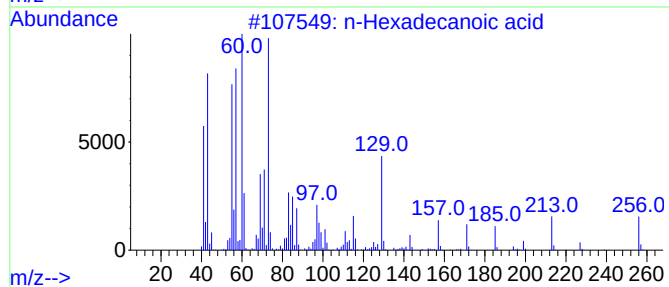
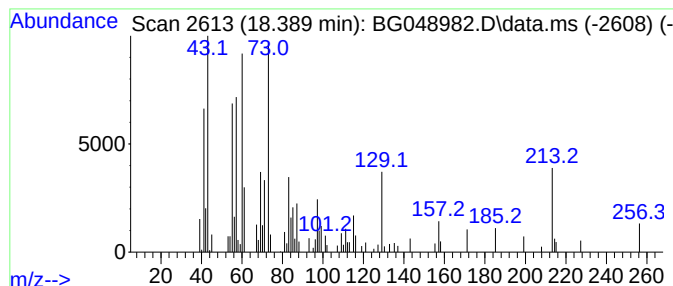
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.390	3.63 ng	97478	Phenanthrene-d10	17.508

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	64
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	62
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5			Undecanoic acid	186	C11H22O2	000112-37-8	50



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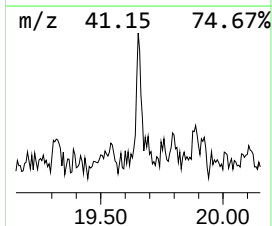
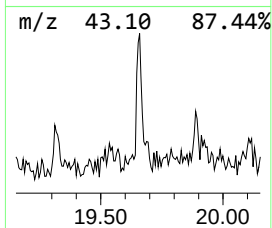
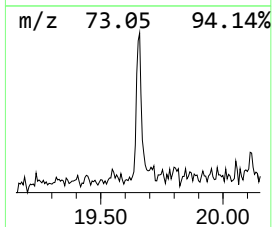
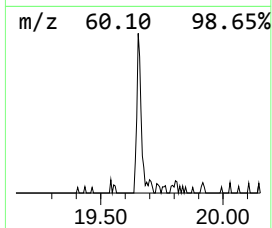
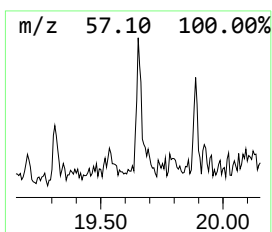
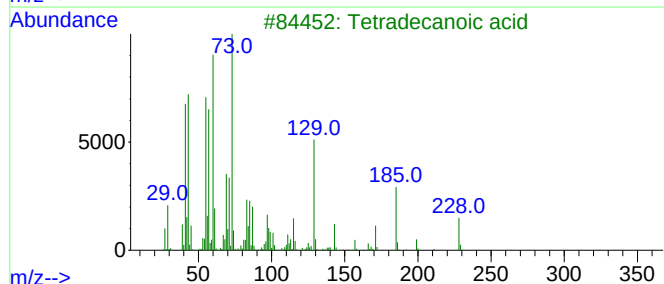
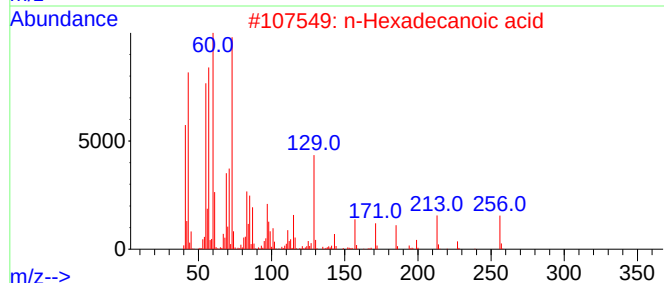
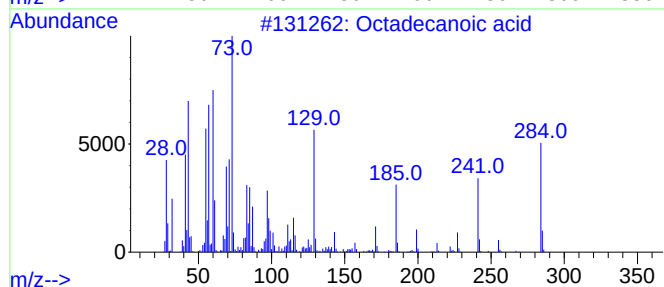
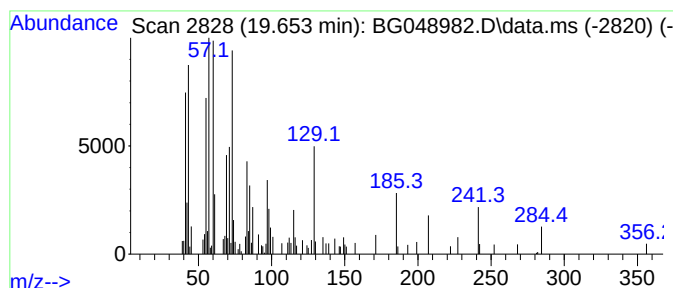
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.653	2.58 ng	87117	Chrysene-d12	21.797

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	94
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	59
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	58
5			Undecanoic acid	186	C11H22O2	000112-37-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048982.D
Acq On : 15 Jun 2021 18:00
Operator : CG/JU
Sample : M2672-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(24-28)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.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
Butane, 2-chlor...	3.160	19.1	ng	206653	1	8.113	216097	20.0
unknown3.284	3.284	6.3	ng	67992	1	8.113	216097	20.0
2-Pentanone, 4-...	5.199	2.9	ng	31749	1	8.113	216097	20.0
Benzene, 1,3-di...	5.734	2.7	ng	29008	1	8.113	216097	20.0
n-Hexadecanoic ...	18.390	3.6	ng	97478	4	17.508	537546	20.0
Octadecanoic acid	19.653	2.6	ng	87117	5	21.797	674997	20.0