

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030122\
 Data File : BG052519.D
 Acq On : 1 Mar 2022 15:05
 Operator : CG/JU
 Sample : N1688-02
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-15

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-BG020722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG052519.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.264	298	302	309	rVB3	13010	18853	1.12%	0.270%
2	5.752	380	385	393	rVB	88649	139467	8.30%	1.999%
3	7.367	653	660	673	rBV2	58754	116520	6.94%	1.670%
4	8.219	796	805	811	rBV	100067	166303	9.90%	2.383%
5	9.394	996	1005	1014	rBV	269351	490270	29.19%	7.026%
6	10.804	1240	1245	1254	rBV2	23642	45214	2.69%	0.648%
7	11.057	1281	1288	1295	rBV	129491	227092	13.52%	3.255%
8	13.489	1694	1702	1712	rBV	704338	1105656	65.83%	15.845%
9	14.481	1867	1871	1880	rBV3	23714	42612	2.54%	0.611%
10	14.787	1918	1923	1930	rBV	22977	45785	2.73%	0.656%
11	14.863	1930	1936	1942	rVB	202023	312027	18.58%	4.472%
12	15.639	2062	2068	2074	rBV2	34263	61840	3.68%	0.886%
13	16.191	2157	2162	2166	rBV2	12388	17674	1.05%	0.253%
14	16.349	2184	2189	2204	rBV	256928	431191	25.67%	6.179%
15	17.066	2305	2311	2316	rBV6	14122	20320	1.21%	0.291%
16	17.336	2352	2357	2363	rBV4	14493	21661	1.29%	0.310%
17	17.495	2379	2384	2390	rBV	57848	77710	4.63%	1.114%
18	17.612	2398	2404	2411	rBV	267541	405921	24.17%	5.817%
19	17.871	2444	2448	2452	rBV	47602	61911	3.69%	0.887%
20	18.253	2510	2513	2518	rVB2	28541	37417	2.23%	0.536%
21	18.552	2559	2564	2568	rVV	83517	101920	6.07%	1.461%
22	18.899	2619	2623	2628	rVB2	27684	31398	1.87%	0.450%
23	19.334	2694	2697	2702	rBV2	19147	25490	1.52%	0.365%
24	19.580	2736	2739	2742	rBV3	18857	19006	1.13%	0.272%
25	19.874	2784	2789	2795	rVB4	21958	43228	2.57%	0.620%
26	20.209	2840	2846	2854	rVB	1303378	1679528	100.00%	24.070%
27	21.108	2996	2999	3004	rBV2	22102	30123	1.79%	0.432%
28	21.161	3004	3008	3012	rVB	20525	27264	1.62%	0.391%
29	21.525	3061	3070	3079	rBV2	48643	111009	6.61%	1.591%
30	21.783	3109	3114	3121	rVB	24585	43244	2.57%	0.620%
31	21.930	3132	3139	3148	rBV	285316	490752	29.22%	7.033%
32	25.396	3718	3729	3741	rBV2	172921	529374	31.52%	7.587%

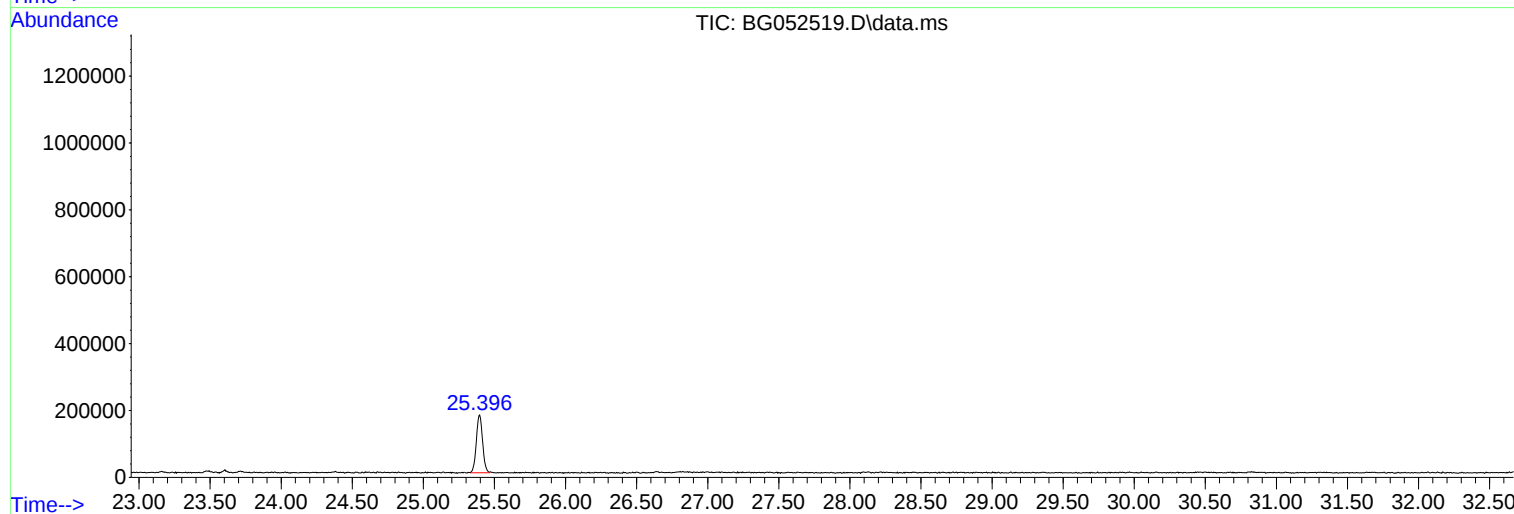
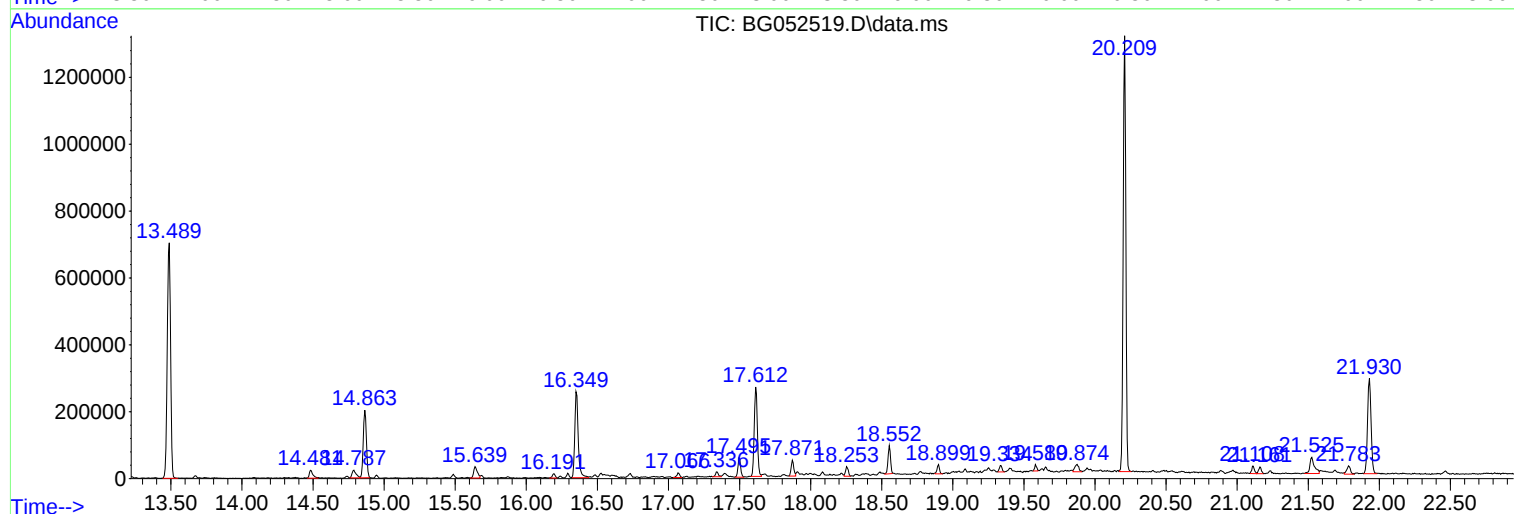
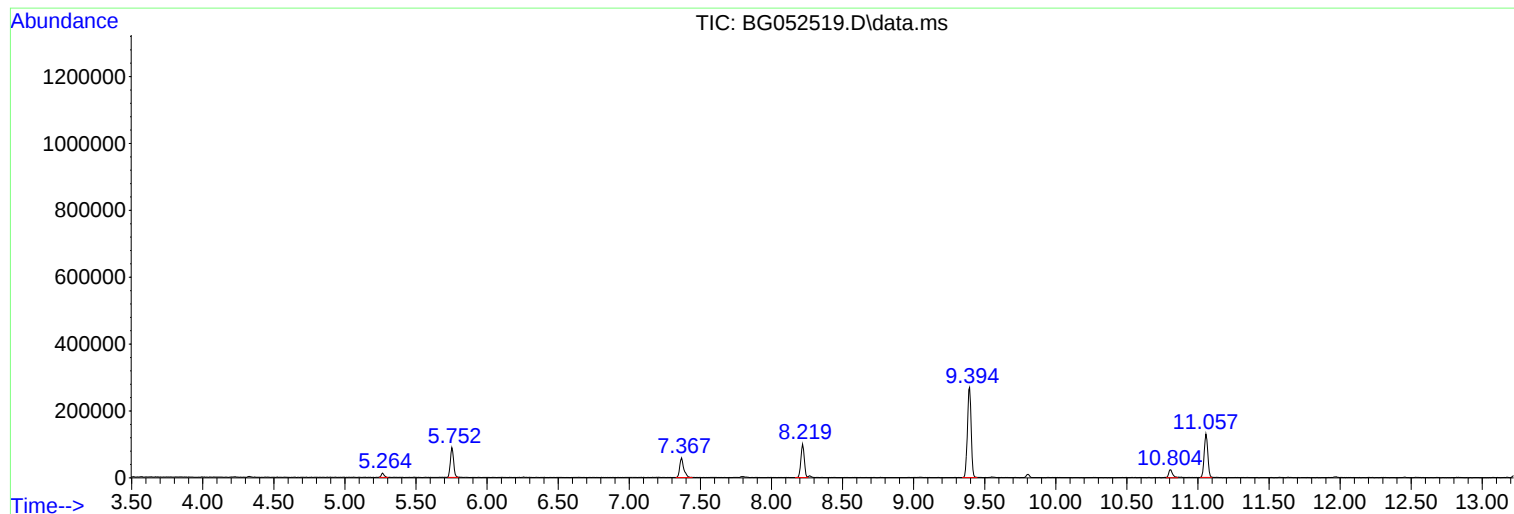
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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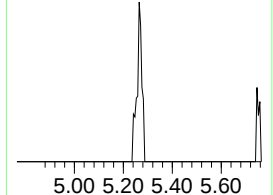
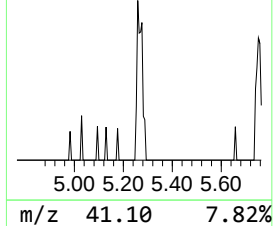
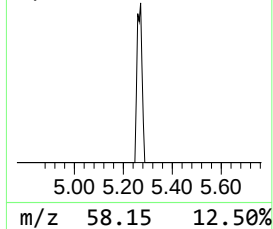
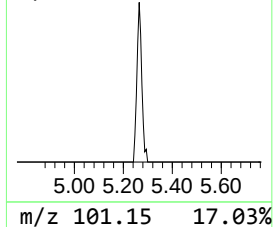
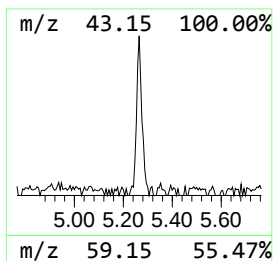
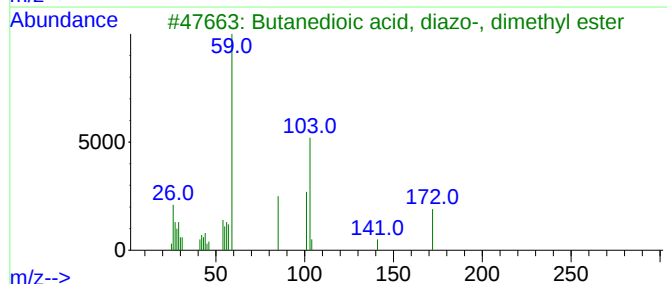
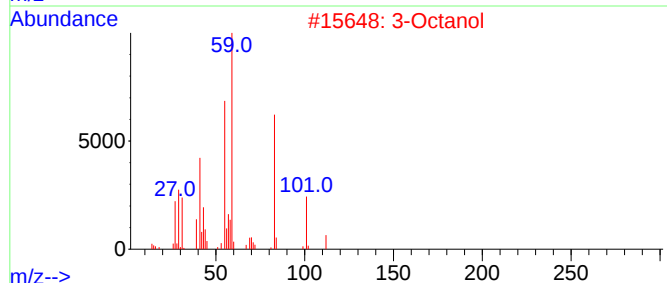
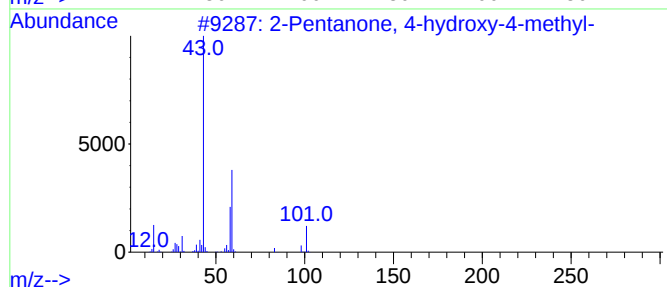
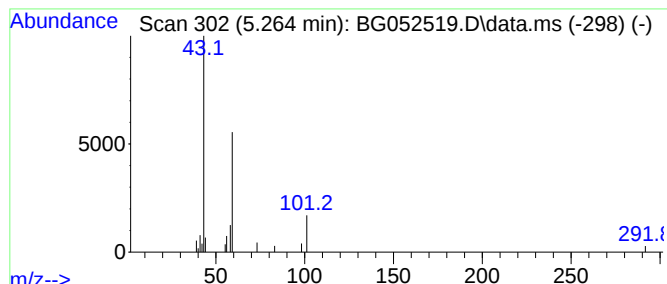
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.264	2.27 ng	18853	1,4-Dichlorobenzene-d4	8.219

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		3-Octanol	130	C8H18O	000589-98-0	33
3		Butanedioic acid, diazo-, dimeth...	172	C6H8N2O4	055514-36-8	25
4		N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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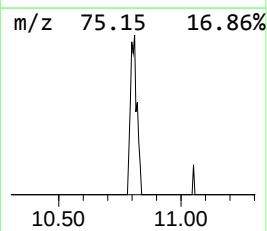
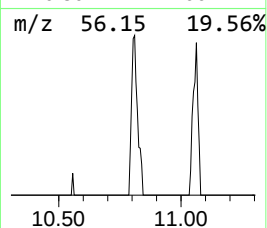
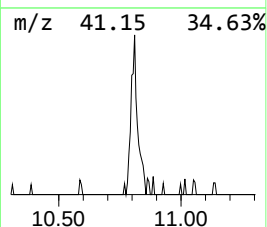
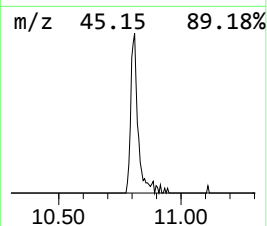
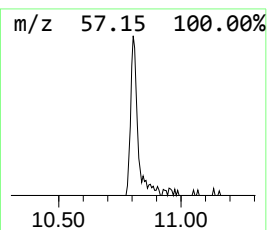
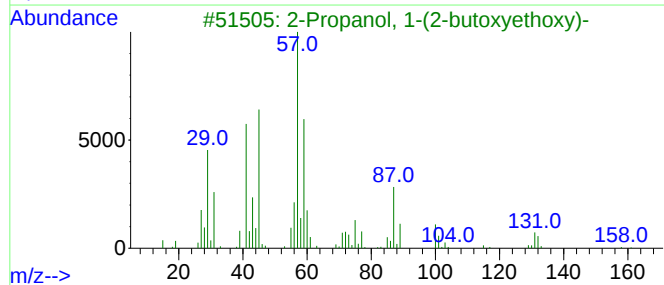
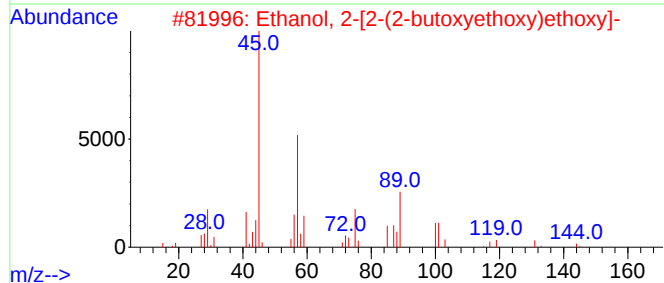
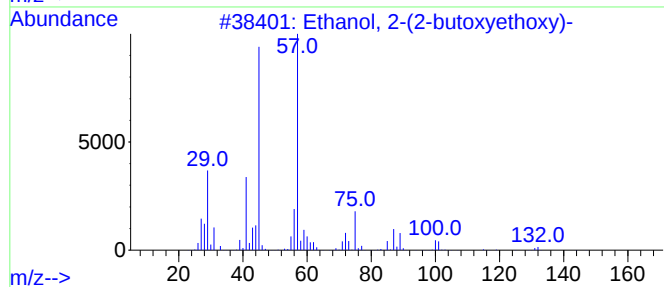
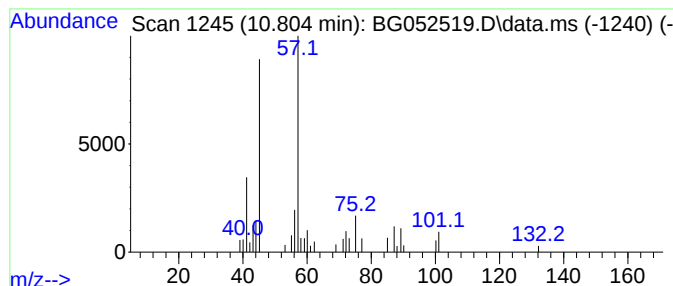
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.804	3.98 ng	45214	Naphthalene-d8	11.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	72
2			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50
3			2-Propanol, 1-(2-butoxyethoxy)-	176	C9H20O3	000124-16-3	45
4			Carbonic acid, bis(1-methylpropy...	174	C9H18O3	000623-63-2	43
5			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	43



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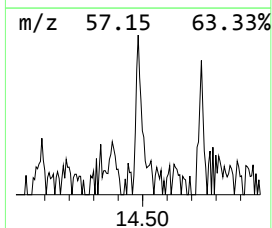
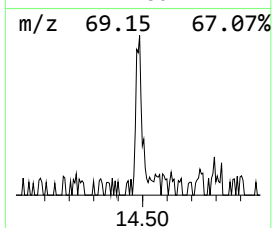
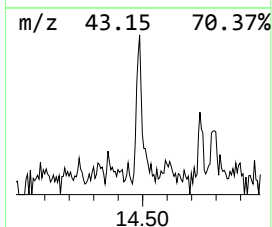
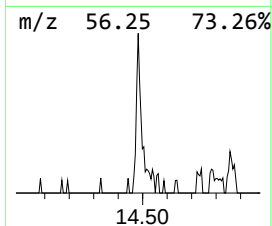
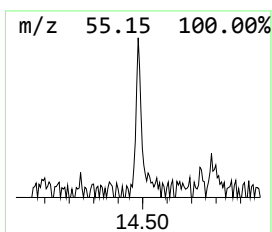
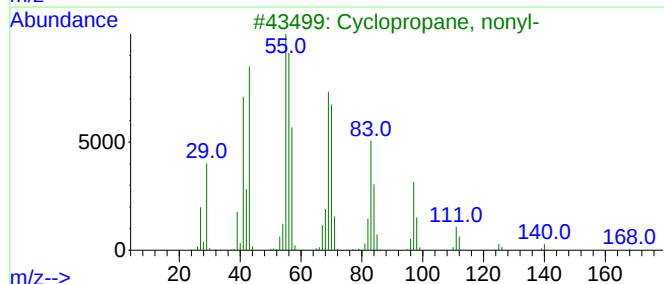
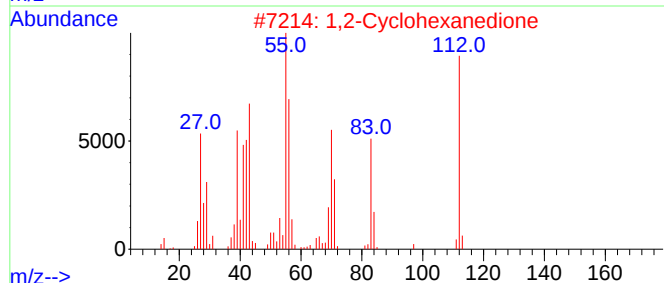
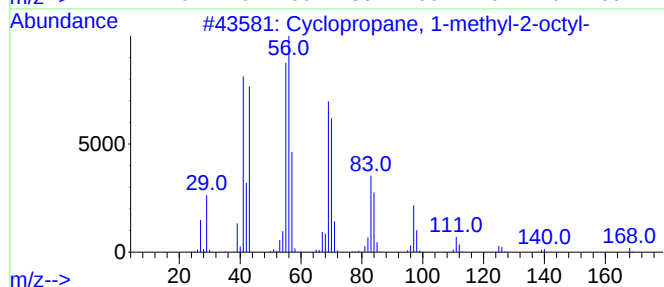
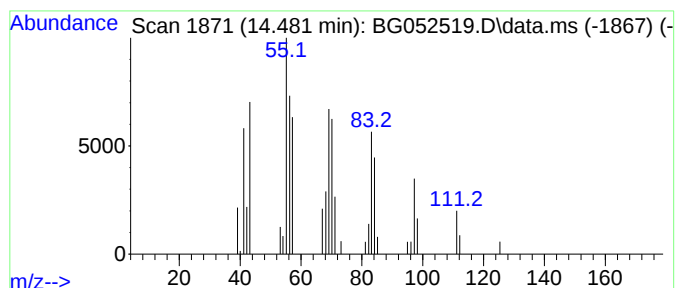
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Cyclopropane, 1-methyl-2-oc... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.481	2.73 ng	42612	Acenaphthene-d10		14.863	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Cyclopropane, 1-methyl-2-octyl-		168	C12H24	037617-26-8	64
2	1,2-Cyclohexanedione		112	C6H8O2	000765-87-7	60
3	Cyclopropane, nonyl-		168	C12H24	074663-85-7	58
4	Cyclopropane, pentyl-		112	C8H16	002511-91-3	58
5	Cyclooctane		112	C8H16	000292-64-8	50



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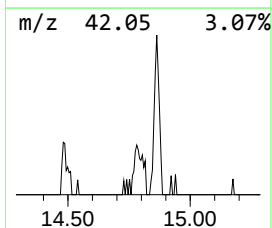
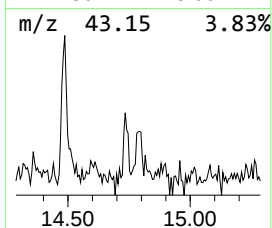
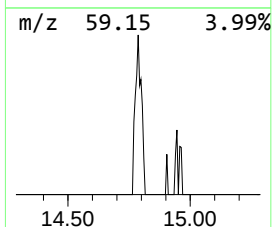
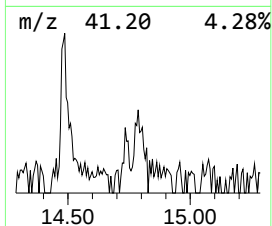
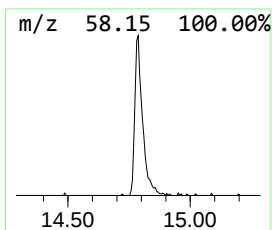
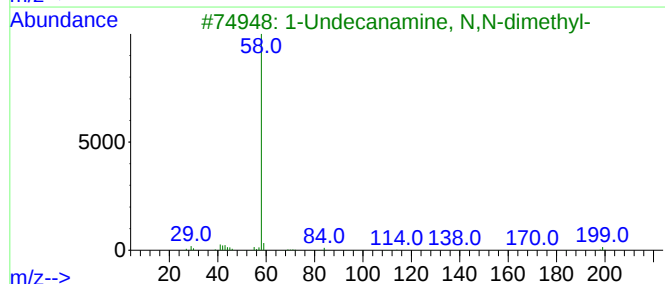
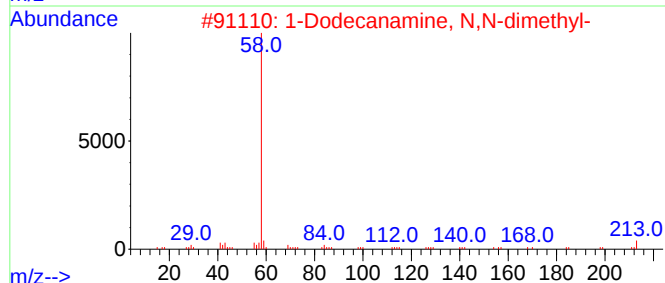
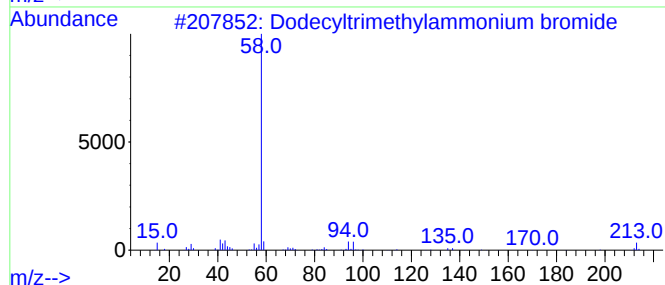
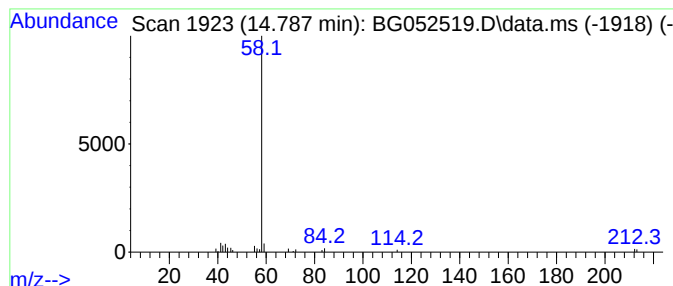
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Dodecyltrimethylammonium br... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.787	2.93 ng	45785	Acenaphthene-d10	14.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecyltrimethylammonium bromide	307	C15H34BrN	001119-94-4	78
2			1-Dodecanamine, N,N-dimethyl-	213	C14H31N	000112-18-5	78
3			1-Undecanamine, N,N-dimethyl-	199	C13H29N	017373-28-3	72
4			1-Tridecanamine, N,N-dimethyl-	227	C15H33N	017373-29-4	72
5			Dimethyl palmitamine	269	C18H39N	000112-69-6	72



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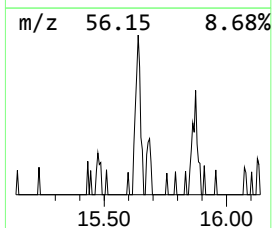
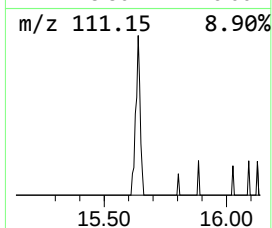
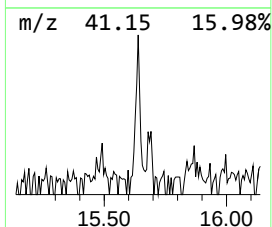
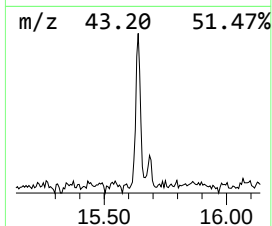
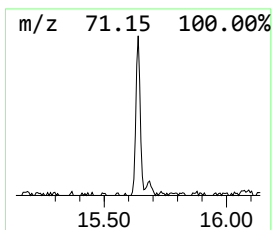
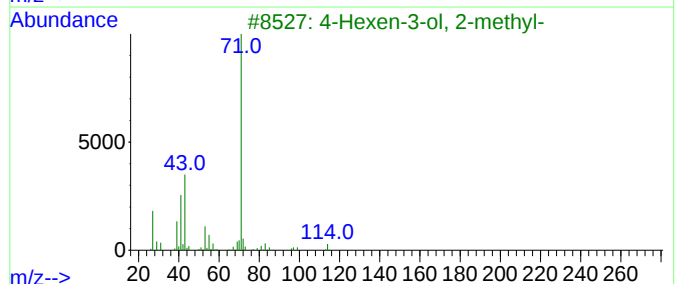
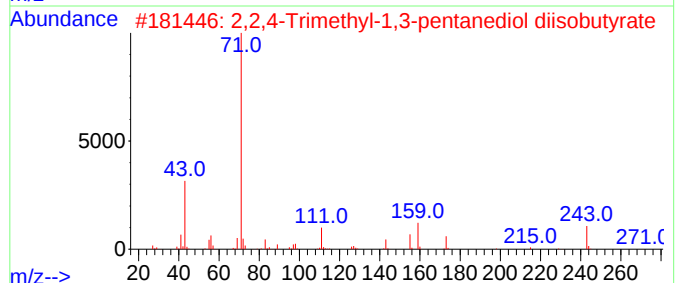
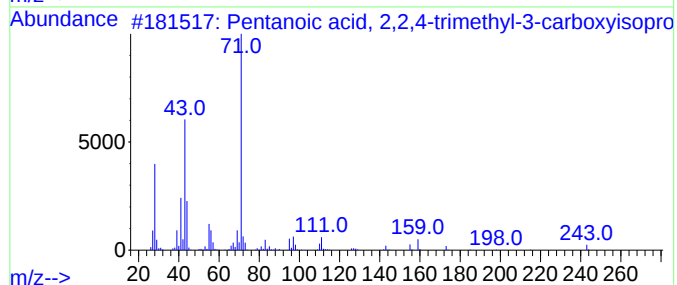
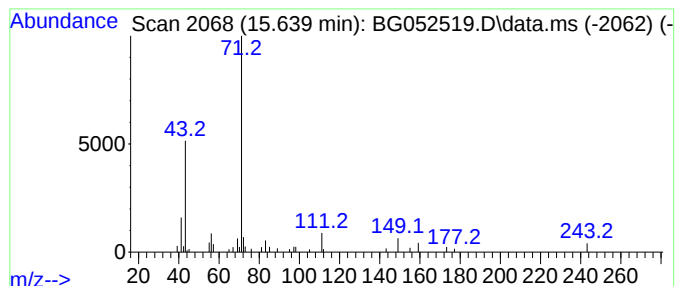
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Peak Number 5 Pentanoic acid, 2,2,4-trime... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.639	3.96 ng	61840	Acenaphthene-d10	14.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanoic acid, 2,2,4-trimethyl-...	286	C16H30O4	1000140-77-5	78
2			2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	78
3			4-Hexen-3-ol, 2-methyl-	114	C7H14O	004798-60-1	53
4			1,2,8-Trimethoxyoctane	204	C11H24O3	062635-58-9	45
5			3-Methyl-hepta-1,6-dien-3-ol	126	C8H14O	034780-69-3	45



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ClientSampleId :
MW-15

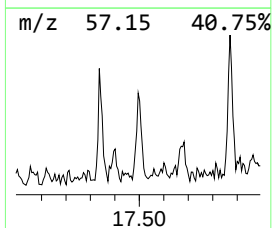
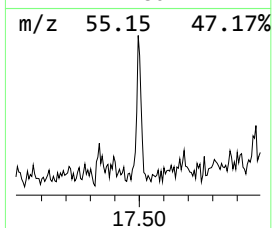
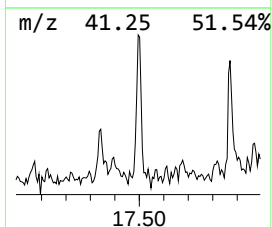
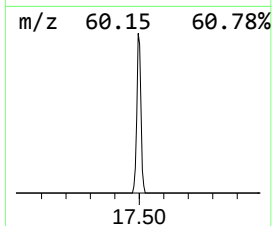
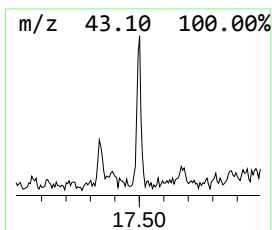
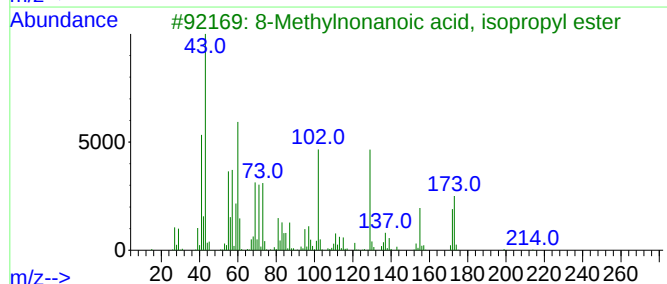
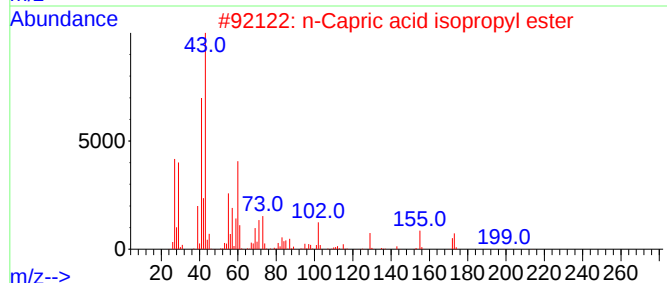
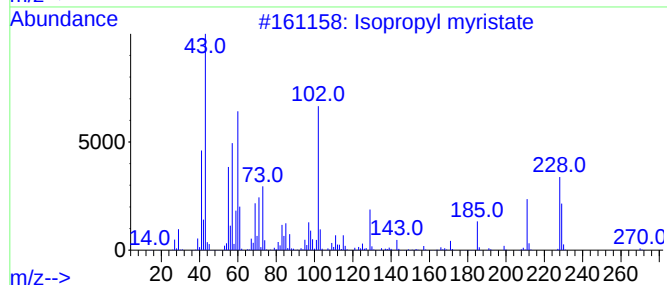
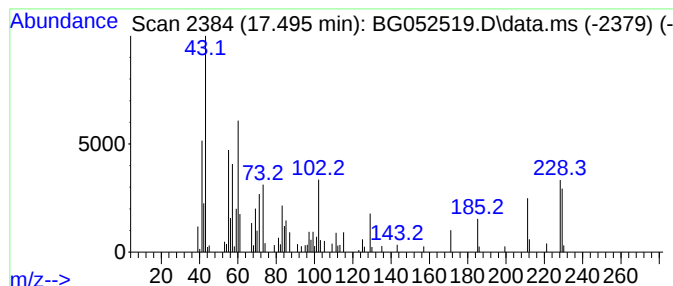
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Isopropyl myristate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.495	3.83 ng	77710	Phenanthrene-d10	17.612

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl myristate	270	C17H34O2	000110-27-0	64
2			n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	46
3			8-Methylnonanoic acid, isopropyl...	214	C13H26O2	1000452-00-6	43
4			Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	43
5			Nonanoic acid, 1-methylethyl ester	200	C12H24O2	028267-32-5	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030122\
Data File : BG052519.D
Acq On : 1 Mar 2022 15:05
Operator : CG/JU
Sample : N1688-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-15

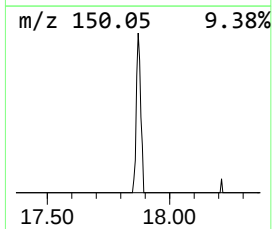
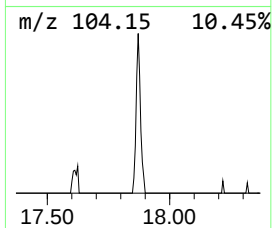
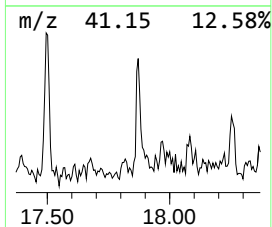
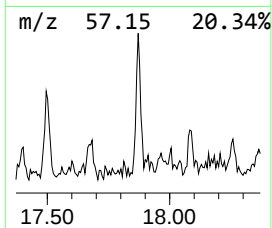
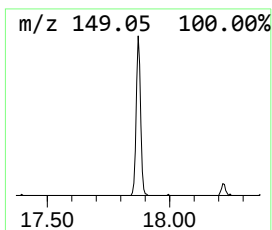
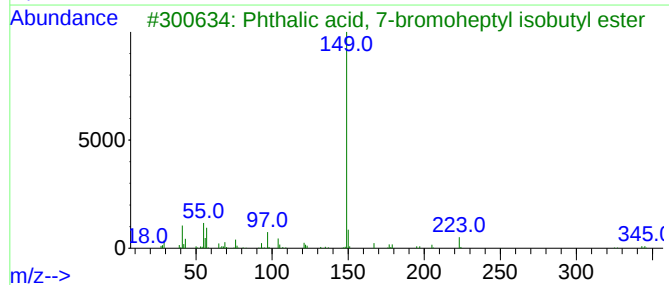
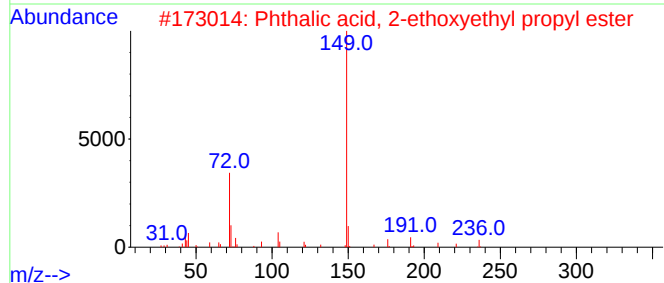
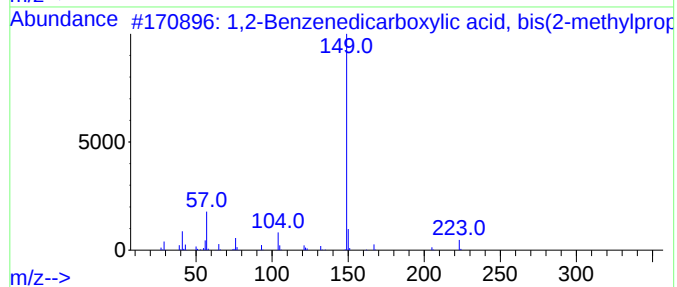
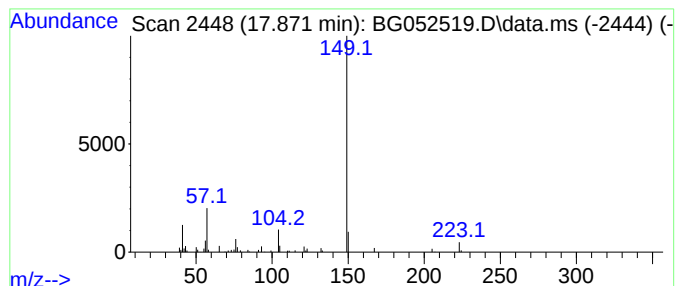
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,2-Benzenedicarboxylic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.871	3.05 ng	61911	Phenanthrene-d10	17.612

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	90
2			Phthalic acid, 2-ethoxyethyl pro...	280	C15H20O5	1000322-87-0	78
3			Phthalic acid, 7-bromoheptyl iso...	398	C19H27BrO4	1000415-51-7	78
4			Dibutyl phthalate	278	C16H22O4	000084-74-2	78
5			Phthalic acid, 2-ethylbutyl isob...	306	C18H26O4	1000356-88-9	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030122\
Data File : BG052519.D
Acq On : 1 Mar 2022 15:05
Operator : CG/JU
Sample : N1688-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

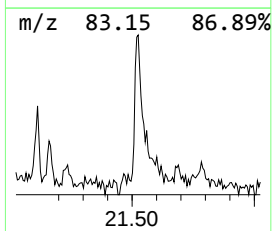
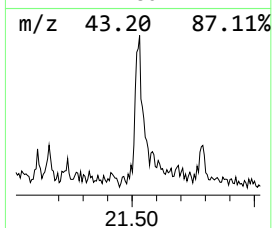
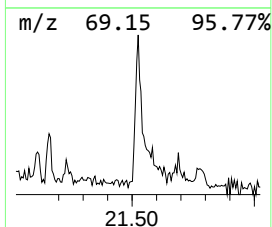
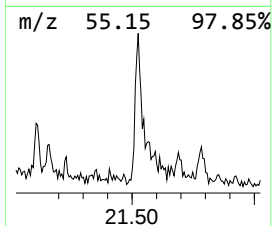
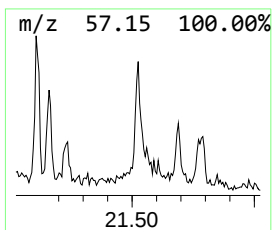
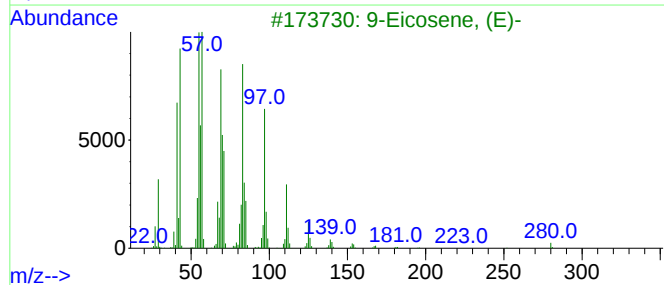
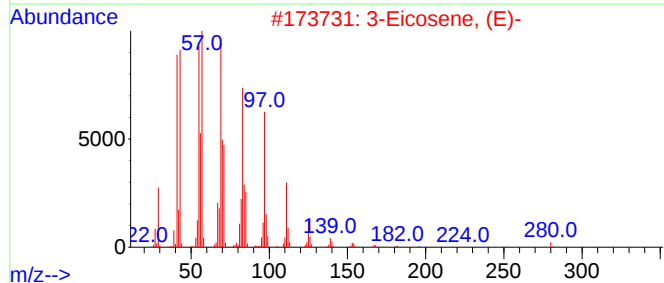
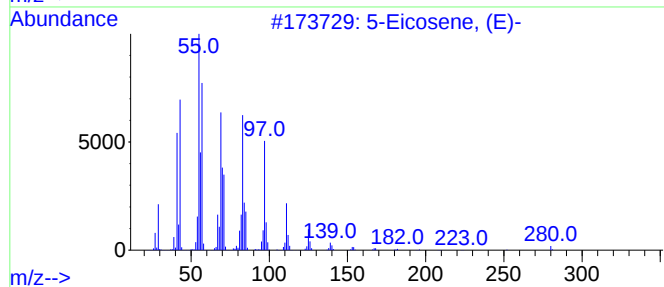
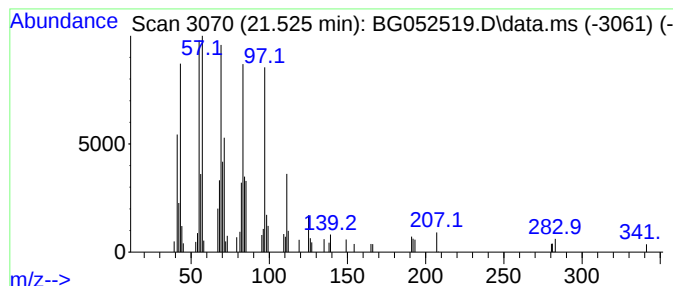
Instrument :
BNA_G
ClientSampleId :
MW-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 5-Eicosene, (E)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.525	4.52 ng	111009	Chrysene-d12	21.930	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	97
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
4	1-Tetracosene	336	C24H48	010192-32-2	91
5	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030122\
Data File : BG052519.D
Acq On : 1 Mar 2022 15:05
Operator : CG/JU
Sample : N1688-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.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-...	5.264	2.3	ng	18853	1	8.219	166303	20.0
Ethanol, 2-(2-b...	10.804	4.0	ng	45214	2	11.057	227092	20.0
Cyclopropane, 1...	14.481	2.7	ng	42612	3	14.863	312027	20.0
Dodecyltrimethy...	14.787	2.9	ng	45785	3	14.863	312027	20.0
Pentanoic acid,...	15.639	4.0	ng	61840	3	14.863	312027	20.0
Isopropyl myris...	17.495	3.8	ng	77710	4	17.612	405921	20.0
1,2-Benzenedica...	17.871	3.0	ng	61911	4	17.612	405921	20.0
5-Eicosene, (E)-	21.525	4.5	ng	111009	5	21.930	490752	20.0