

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032521\
 Data File : BG048511.D
 Acq On : 25 Mar 2021 21:07
 Operator : CG/JU
 Sample : M1796-02
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB-2021-WW-000-06

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-BG031821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048511.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.533	196	203	210	rBV2	25507	44366	2.50%	0.423%
2	4.786	239	246	257	rBV	192080	337394	19.05%	3.220%
3	5.180	308	313	317	rBV2	17396	25626	1.45%	0.245%
4	5.650	385	393	400	rBV	281743	444408	25.09%	4.242%
5	7.254	659	666	675	rVB	229061	400379	22.60%	3.822%
6	8.100	803	810	816	rBV	175277	306801	17.32%	2.928%
7	8.153	816	819	826	rVB3	16608	24409	1.38%	0.233%
8	9.263	999	1008	1016	rBV2	256748	473545	26.73%	4.520%
9	10.244	1171	1175	1187	rVB5	22001	41494	2.34%	0.396%
10	10.920	1283	1290	1299	rVB	232203	411586	23.23%	3.929%
11	11.701	1416	1423	1430	rBV3	25746	46209	2.61%	0.441%
12	11.831	1435	1445	1453	rBV	175074	357819	20.20%	3.415%
13	13.006	1638	1645	1648	rBV3	13655	20759	1.17%	0.198%
14	13.364	1698	1706	1712	rBV	672397	1072665	60.55%	10.239%
15	14.181	1841	1845	1852	rVB	19225	30945	1.75%	0.295%
16	14.739	1934	1940	1948	rVB	375914	586203	33.09%	5.595%
17	15.139	2003	2008	2013	rBV2	33560	48350	2.73%	0.462%
18	16.226	2186	2193	2199	rBV	690332	1040398	58.73%	9.931%
19	17.489	2401	2408	2415	rVB	479570	740509	41.80%	7.068%
20	18.370	2553	2558	2563	rBV2	84225	118761	6.70%	1.134%
21	19.498	2746	2750	2752	rBV3	13604	22475	1.27%	0.215%
22	19.639	2770	2774	2780	rBV7	39799	56522	3.19%	0.540%
23	20.098	2845	2852	2858	rBV	1396291	1771413	100.00%	16.908%
24	21.414	3071	3076	3085	rBV7	49594	111735	6.31%	1.067%
25	21.784	3132	3139	3147	rVB2	474235	805158	45.45%	7.685%
26	23.170	3367	3375	3382	rBV5	55698	196697	11.10%	1.877%
27	23.523	3428	3435	3443	rVB2	39440	85836	4.85%	0.819%
28	25.109	3695	3705	3722	rBV2	279911	854164	48.22%	8.153%

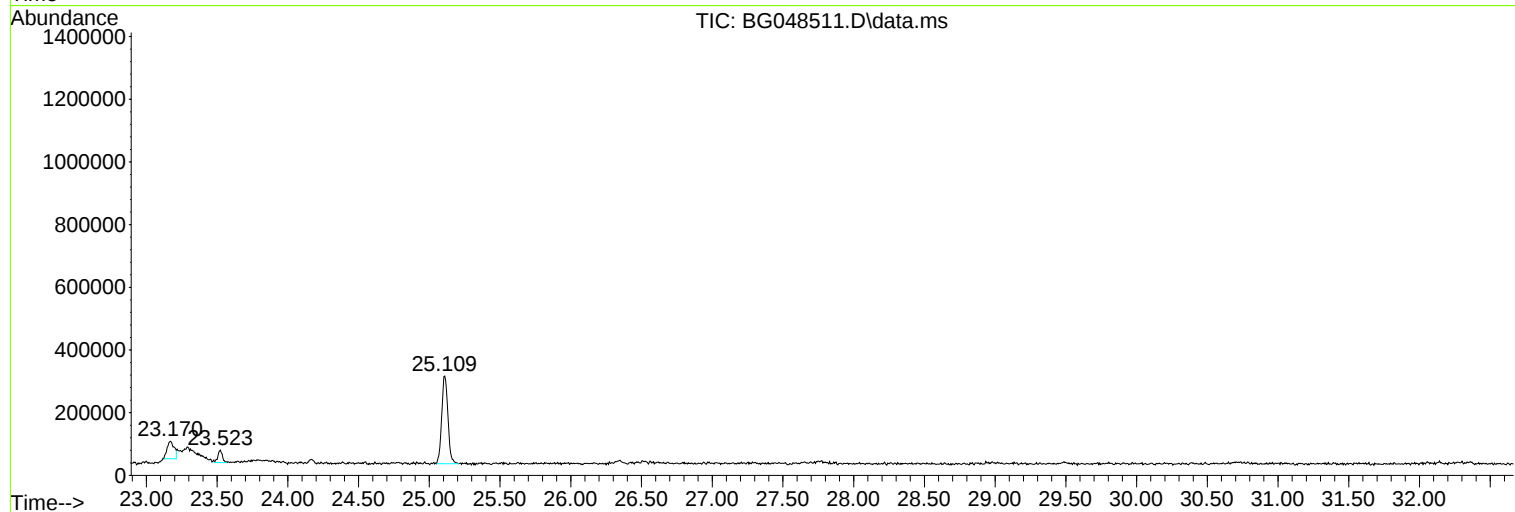
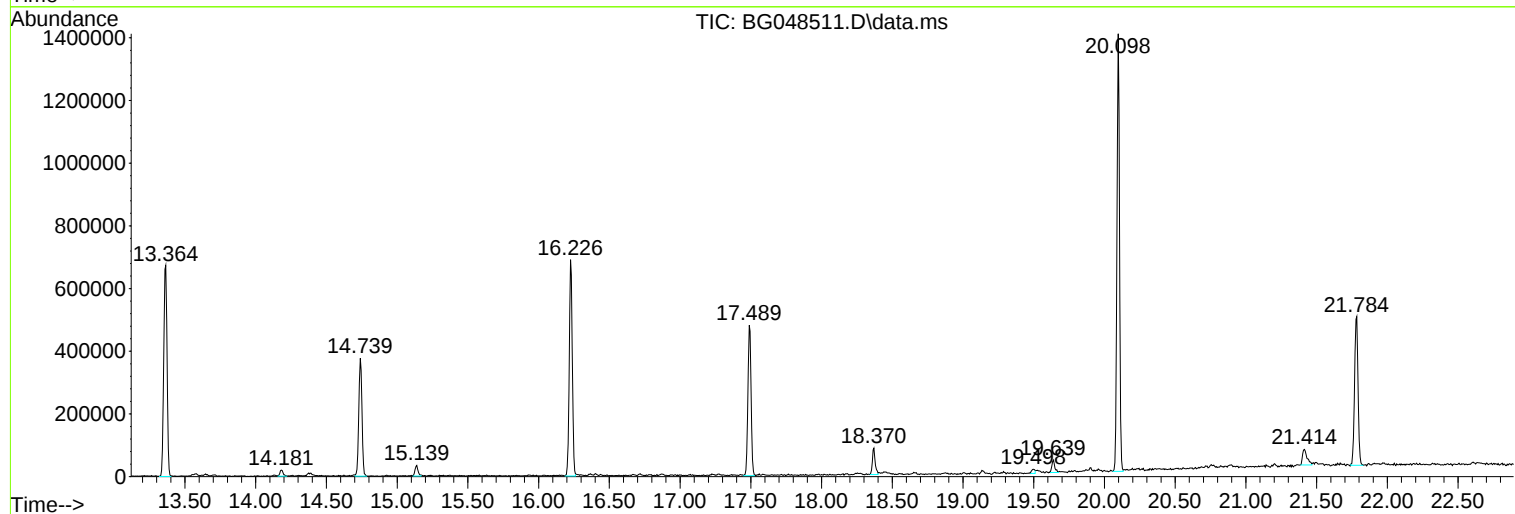
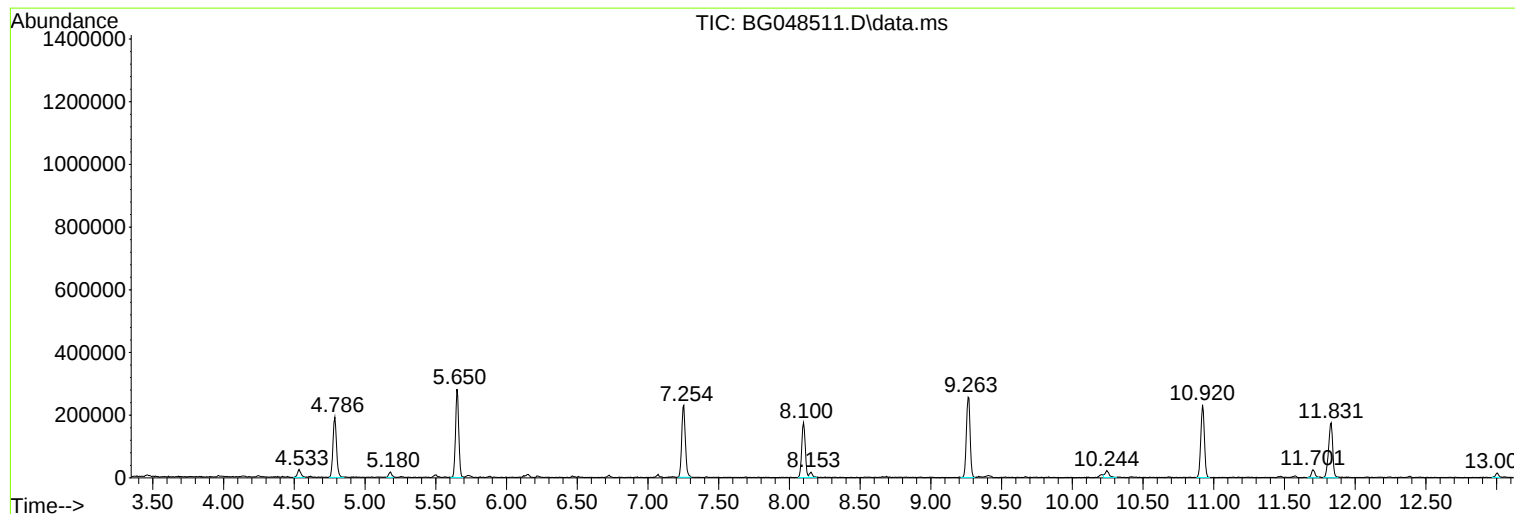
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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.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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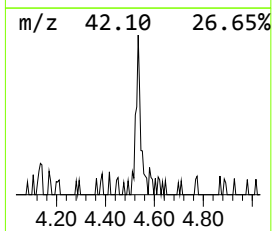
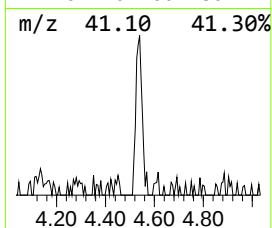
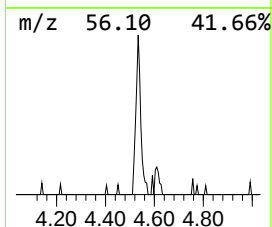
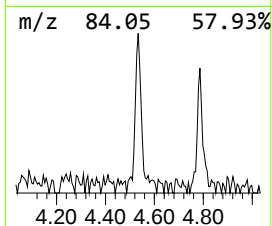
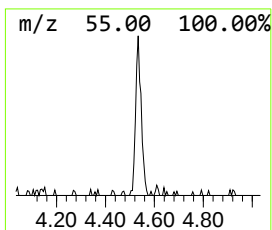
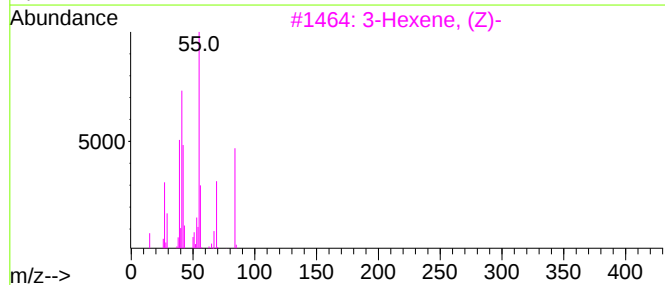
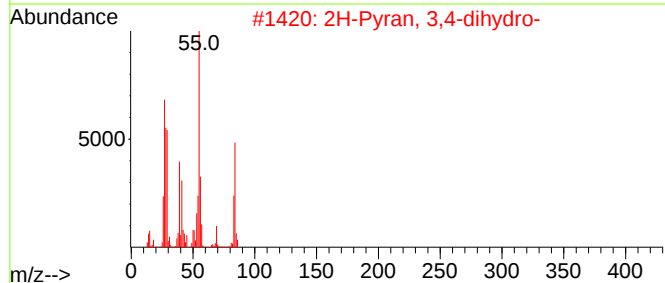
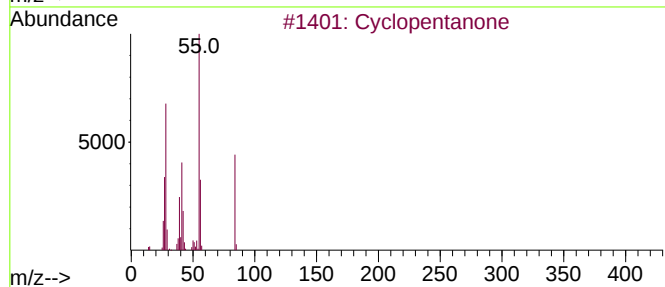
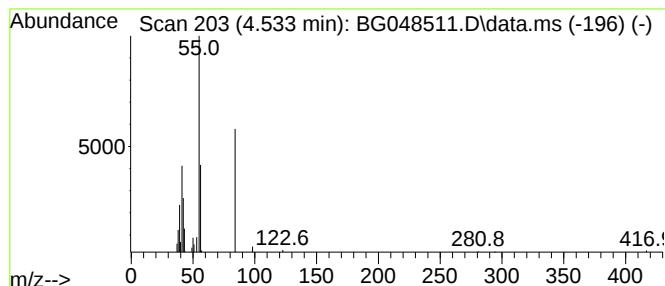
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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Peak Number 1 Cyclopentanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.533	2.89 ng	44366	1,4-Dichlorobenzene-d4	8.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentanone	84	C5H8O	000120-92-3	83
2			2H-Pyran, 3,4-dihydro-	84	C5H8O	000110-87-2	45
3			3-Hexene, (Z)-	84	C6H12	007642-09-3	42
4			2-Pentenal, (E)-	84	C5H8O	001576-87-0	38
5			Cyclopentanone, 2-ethyl-	112	C7H12O	004971-18-0	33



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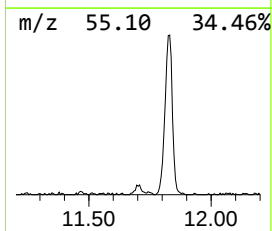
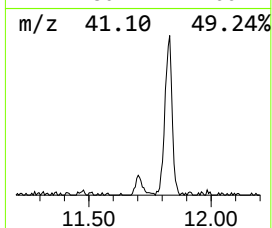
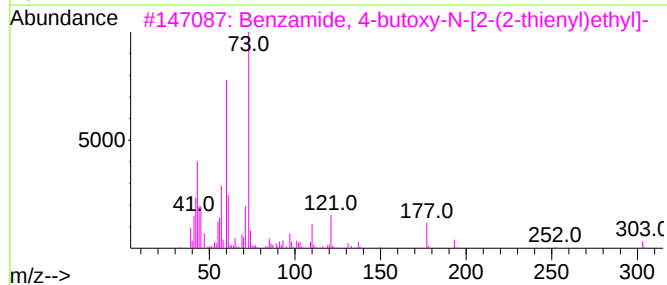
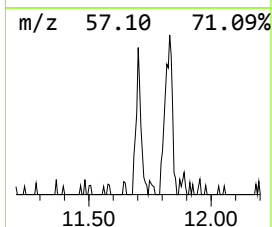
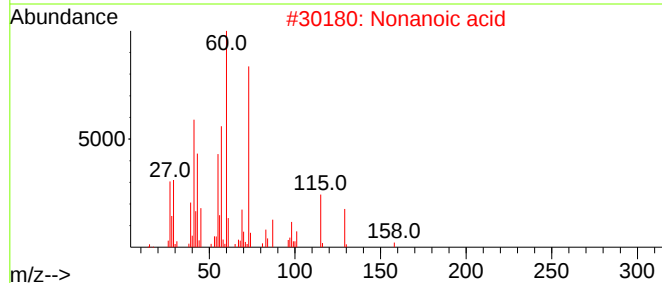
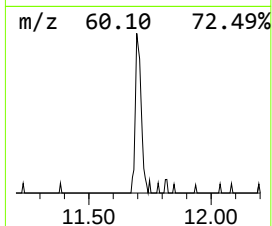
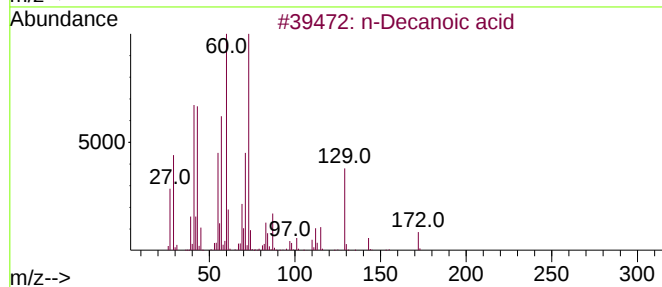
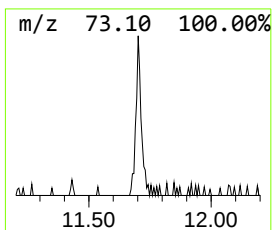
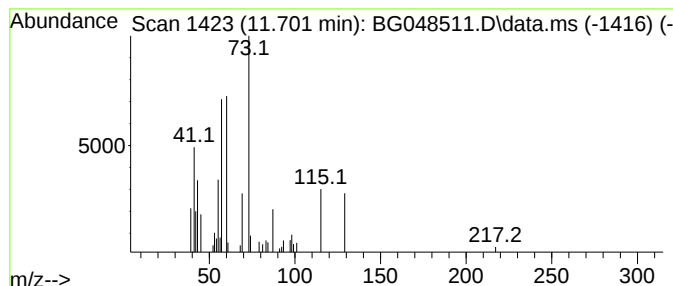
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Peak Number 3 n-Decanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.701	2.25 ng	46209	Naphthalene-d8	10.920

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Decanoic acid	172	C10H20O2	000334-48-5	53
2			Nonanoic acid	158	C9H18O2	000112-05-0	40
3			Benzamide, 4-butoxy-N-[2-(2-thie...	303	C17H21NO2S	1000319-87-5	38
4			Methyl 3-methyl-3-(methoxy-isopr...	219	C10H21NO4	082004-48-6	38
5			D-Mannoheptulose	210	C7H14O7	003615-44-9	32



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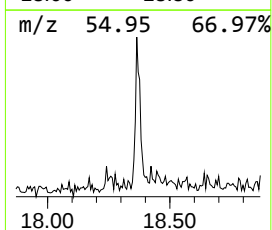
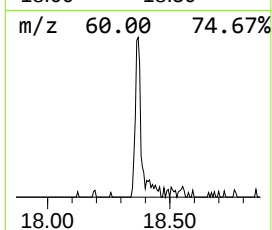
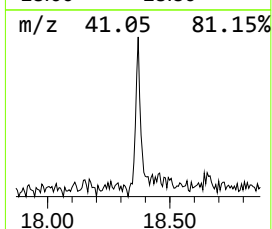
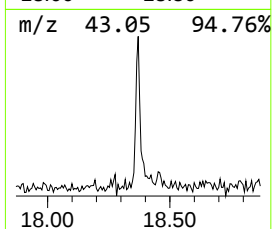
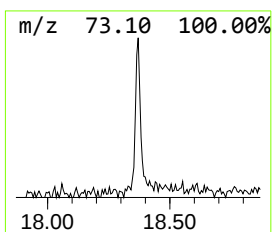
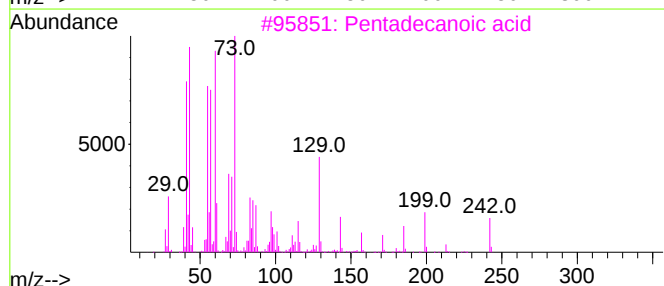
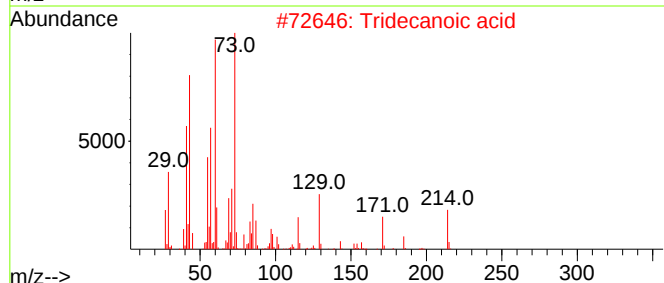
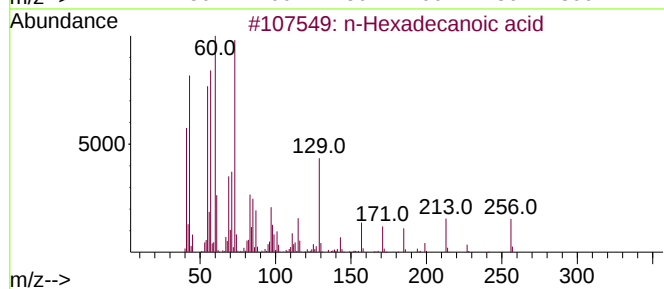
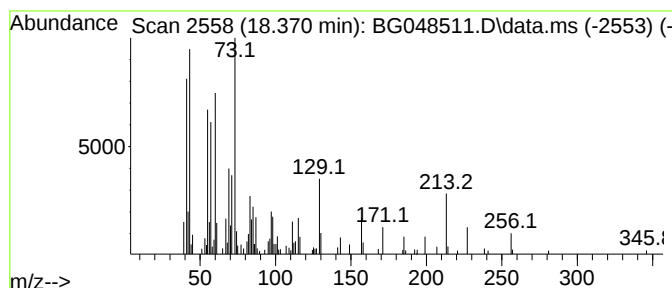
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BNA_G
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.370	3.21 ng	118761	Phenanthrene-d10		17.489	
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	89
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	53
4	Dodecanoic acid		200	C12H24O2	000143-07-7	53
5	Tetradecanoic acid		228	C14H28O2	000544-63-8	53



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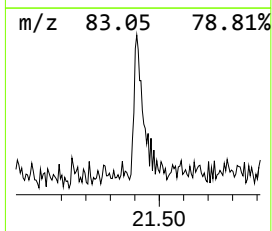
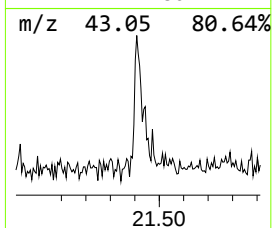
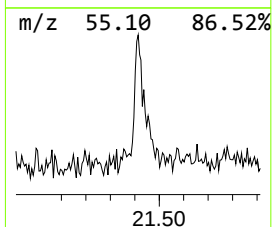
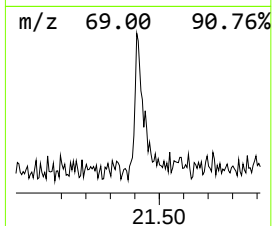
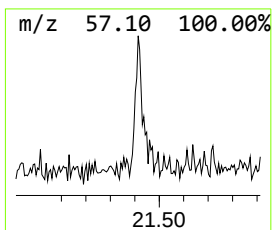
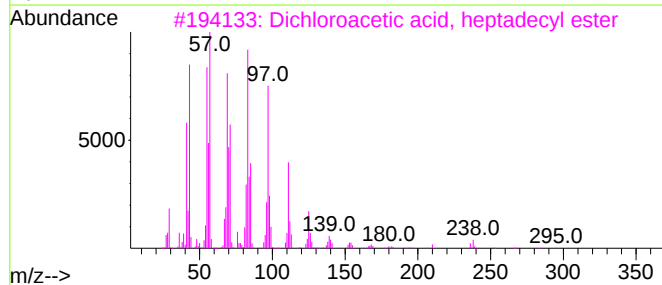
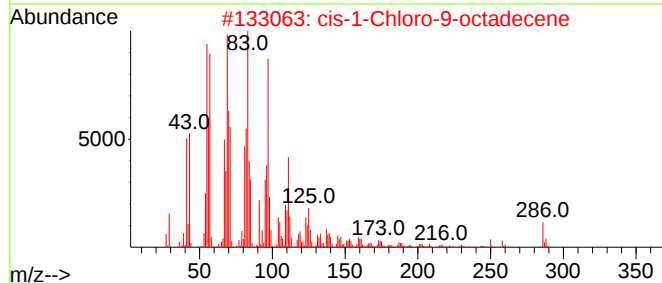
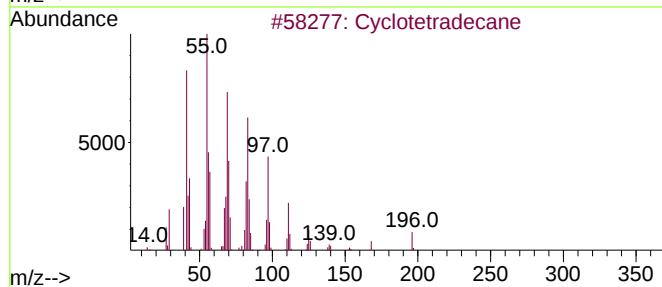
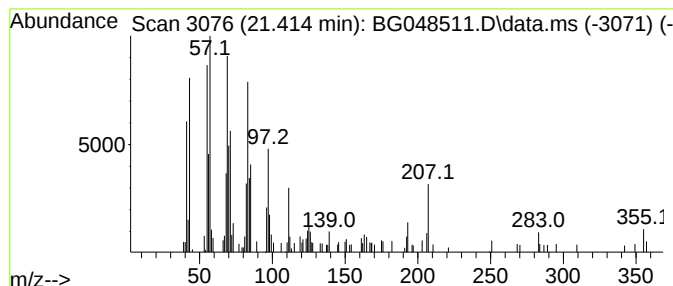
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Peak Number 5 Cyclotetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.414	2.78 ng	111735	Chrysene-d12	21.784

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetradecane	196	C14H28	000295-17-0	93
2			cis-1-Chloro-9-octadecene	286	C18H35Cl	016507-61-2	89
3			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	81
4			Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	81
5			Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	74



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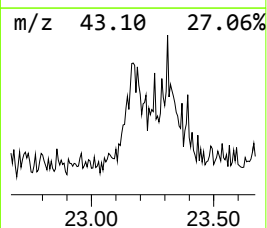
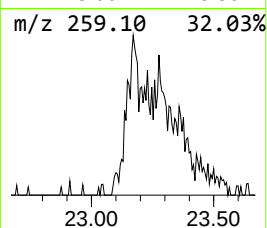
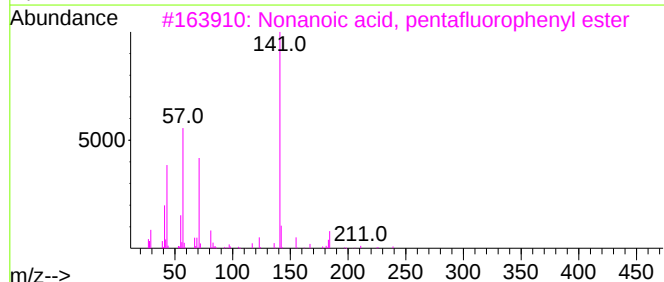
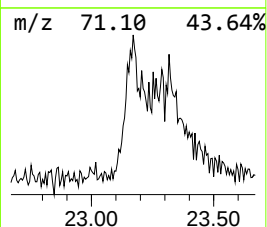
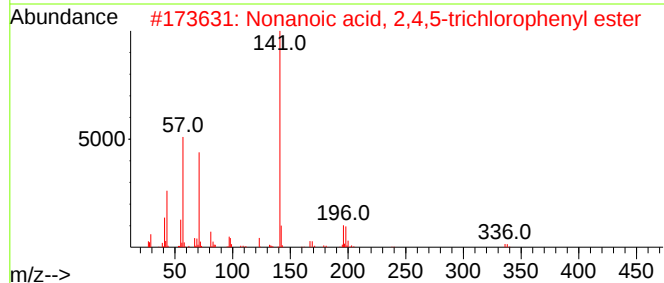
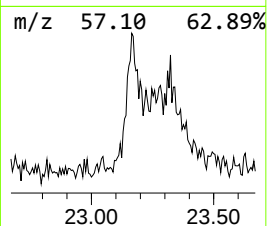
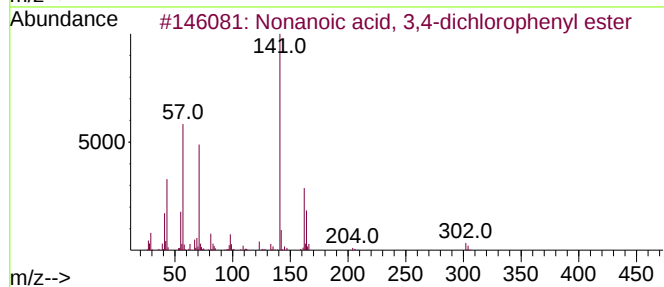
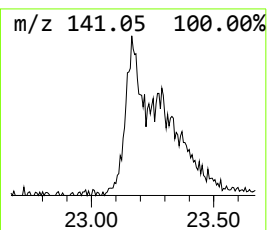
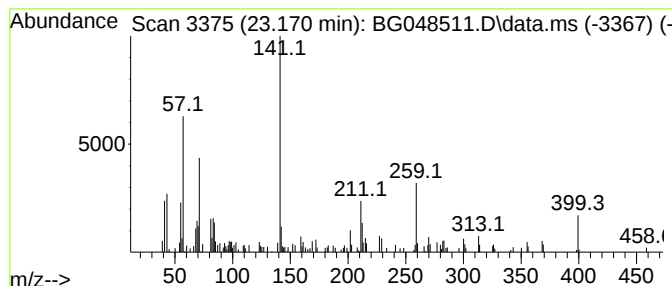
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 unknown23.170 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.170	4.89 ng	196697	Chrysene-d12	21.784

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanoic acid, 3,4-dichloropheny...	302	C15H20Cl2O2	1000358-02-7	47
2			Nonanoic acid, 2,4,5-trichloroph...	336	C15H19Cl3O2	1000360-67-3	47
3			Nonanoic acid, pentafluorophenyl...	324	C15H17F5O2	1000360-66-5	47
4			3-Methyl-thiophene-2-carboxamide	141	C6H7NOS	076655-99-7	38
5			2,4-Difluorobenzamide, N-pentyl-	227	C12H15F2NO	1000358-05-3	35



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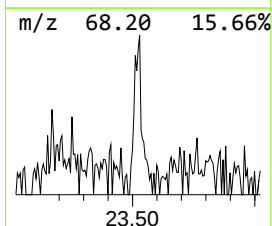
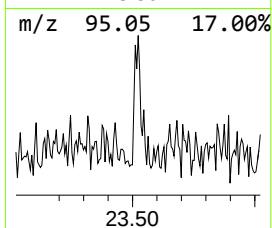
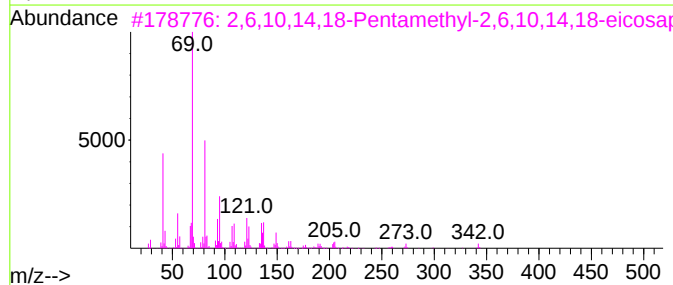
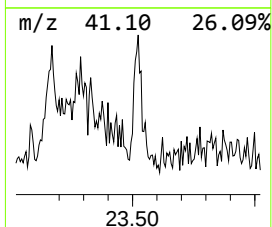
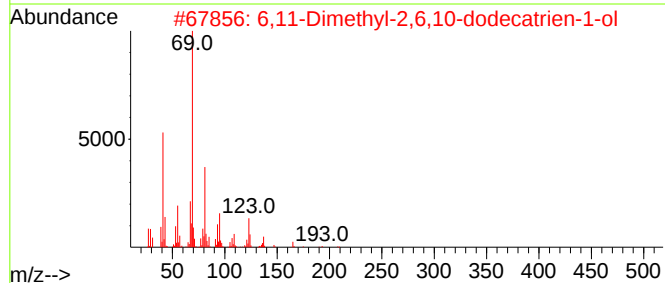
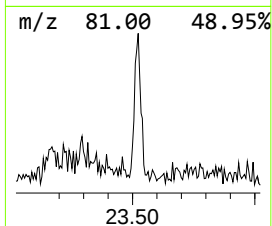
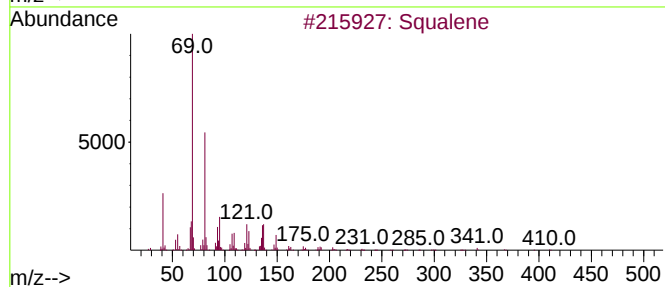
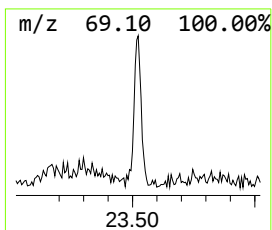
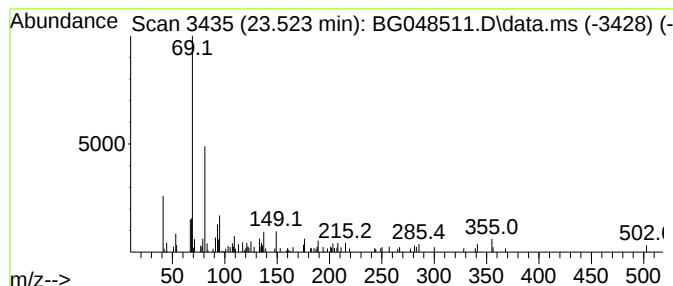
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.523	2.01 ng	85836	Perylene-d12	25.109

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	56
2			6,11-Dimethyl-2,6,10-dodecatrien...	208	C14H24O	1000196-53-3	45
3			2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	45
4			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	42
5			Farnesol isomer a	222	C15H26O	1000108-92-4	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032521\
Data File : BG048511.D
Acq On : 25 Mar 2021 21:07
Operator : CG/JU
Sample : M1796-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB-2021-WW-000-06

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.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
Cyclopentanone	4.533	2.9	ng	44366	1	8.100	306801	20.0
n-Decanoic acid	11.701	2.3	ng	46209	2	10.920	411586	20.0
n-Hexadecanoic ...	18.370	3.2	ng	118761	4	17.489	740509	20.0
Cyclotetradecane	21.414	2.8	ng	111735	5	21.784	805158	20.0
unknown23.170	23.170	4.9	ng	196697	5	21.784	805158	20.0
Squalene	23.523	2.0	ng	85836	6	25.109	854164	20.0