

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110323\
 Data File : BF136135.D
 Acq On : 03 Nov 2023 20:42
 Operator : CG\JU
 Sample : 05213-02
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ETGI-293

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_F\Methods\8270-BF103023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136135.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.046	493	503	510	rBV	37926	49641	3.26%	0.361%
2	5.446	566	571	574	rBV	1614442	1394476	91.51%	10.137%
3	6.446	736	741	744	rBV	1409251	1333646	87.52%	9.695%
4	6.646	772	775	782	rBV	30234	32703	2.15%	0.238%
5	6.816	801	804	808	rBV	635525	511165	33.55%	3.716%
6	7.375	895	899	902	rBV	989889	885156	58.09%	6.435%
7	8.098	1018	1022	1025	rBV	831211	633913	41.60%	4.608%
8	9.175	1202	1205	1208	rBV	1931657	1523809	100.00%	11.077%
9	9.298	1222	1226	1230	rBV	969774	823750	54.06%	5.988%
10	9.857	1317	1321	1324	rVB	761555	632269	41.49%	4.596%
11	10.645	1451	1455	1458	rBV	982215	824009	54.08%	5.990%
12	11.345	1570	1574	1577	rBV	694774	569840	37.40%	4.142%
13	11.369	1577	1578	1581	rVB	65519	38802	2.55%	0.282%
14	11.751	1640	1643	1649	rVB2	27415	24092	1.58%	0.175%
15	11.886	1662	1666	1669	rBV2	181205	165361	10.85%	1.202%
16	11.922	1669	1672	1676	rVB	70531	65228	4.28%	0.474%
17	12.445	1757	1761	1762	rBV2	22874	23760	1.56%	0.173%
18	12.463	1762	1764	1767	rVB	105737	86433	5.67%	0.628%
19	12.563	1776	1781	1785	rBV	95341	91415	6.00%	0.665%
20	12.610	1786	1789	1792	rVV	37961	33973	2.23%	0.247%
21	12.680	1796	1801	1804	rVV2	99223	105222	6.91%	0.765%
22	12.716	1804	1807	1810	rVV	305092	282072	18.51%	2.050%
23	12.775	1814	1817	1818	rVV	41360	33795	2.22%	0.246%
24	12.792	1818	1820	1823	rVB	87838	73163	4.80%	0.532%
25	12.945	1842	1846	1850	rBV	1549469	1316407	86.39%	9.569%
26	13.186	1884	1887	1891	rBV2	24885	25001	1.64%	0.182%
27	13.433	1919	1929	1932	rBV9	30984	72612	4.77%	0.528%
28	13.486	1935	1938	1941	rVV2	40484	50725	3.33%	0.369%
29	13.533	1943	1946	1949	rVB2	41292	42399	2.78%	0.308%
30	13.869	2000	2003	2004	rBV	28127	22654	1.49%	0.165%
31	13.892	2004	2007	2019	rVB9	25782	66883	4.39%	0.486%
32	14.004	2021	2026	2029	rBV	711771	714594	46.90%	5.195%
33	14.027	2029	2030	2033	rVB	46865	23734	1.56%	0.173%
34	14.186	2054	2057	2061	rVB	40591	32829	2.15%	0.239%
35	14.492	2106	2109	2112	rBV	41600	42692	2.80%	0.310%
36	14.651	2133	2136	2141	rBV2	31182	44092	2.89%	0.321%

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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

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37	14.792	2156	2160	2161	rBV4	15420	22384	1.47%	0.163%
38	14.810	2161	2163	2167	rVB2	47056	41965	2.75%	0.305%
39	15.051	2199	2204	2207	rBV3	35051	55886	3.67%	0.406%
40	15.163	2219	2223	2227	rVB	37341	42387	2.78%	0.308%
41	15.357	2253	2256	2261	rVB	24341	31930	2.10%	0.232%
42	15.421	2261	2267	2273	rBV	34107	44892	2.95%	0.326%
43	15.492	2273	2279	2287	rVV	582680	715960	46.98%	5.205%
44	15.557	2287	2290	2297	rVB4	23552	33795	2.22%	0.246%
45	16.015	2363	2368	2373	rBV3	20701	33193	2.18%	0.241%
46	16.986	2529	2533	2540	rVB3	10899	22221	1.46%	0.162%
47	17.439	2605	2610	2617	rVB	8992	19390	1.27%	0.141%

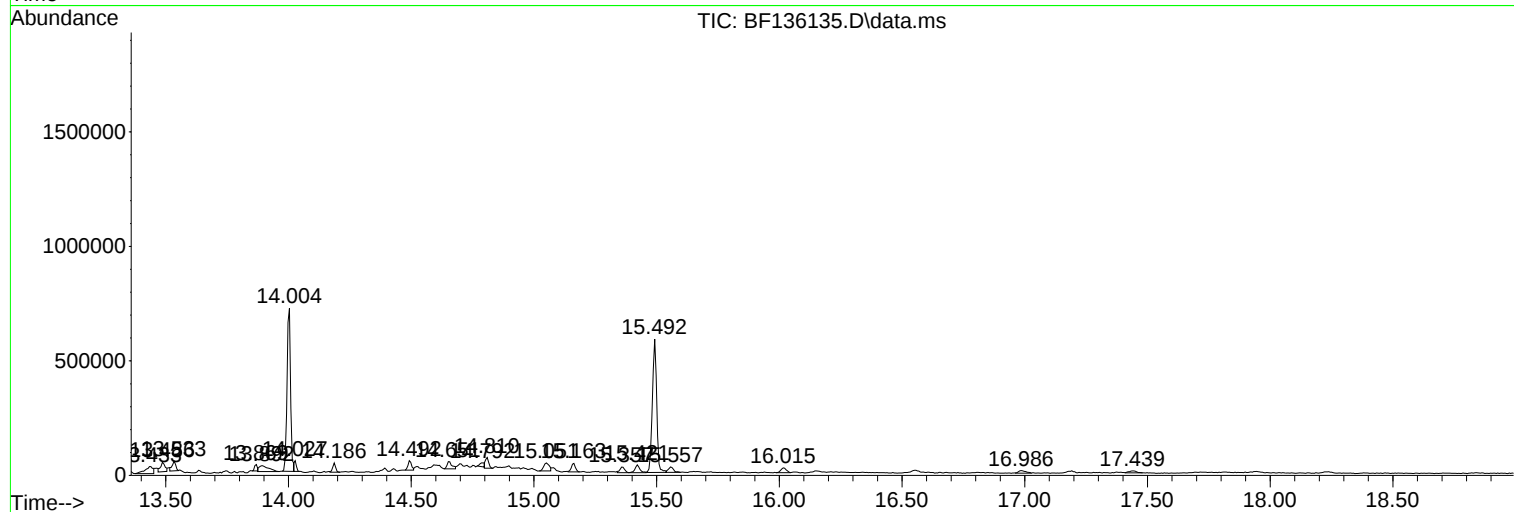
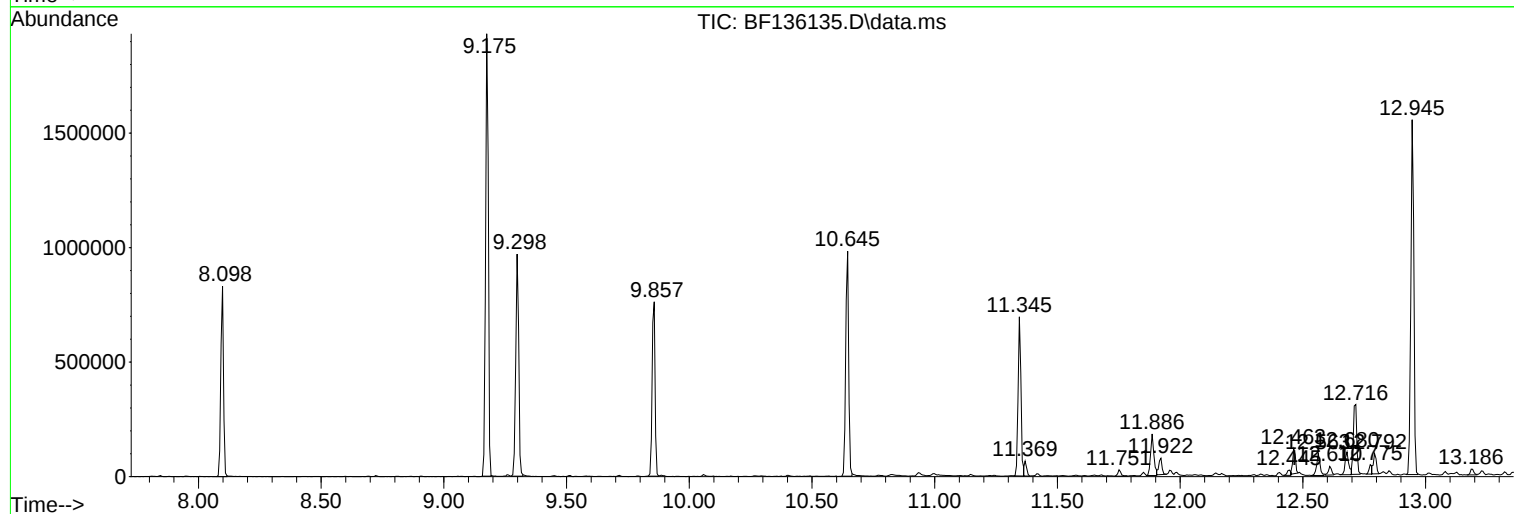
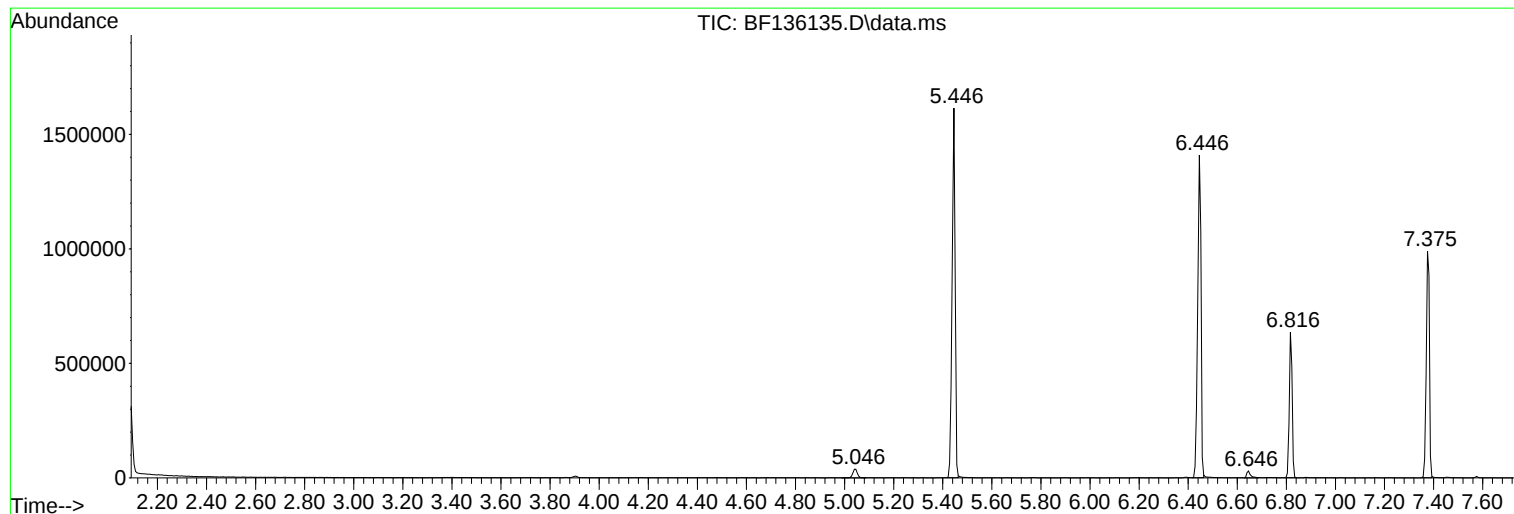
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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ALS Vial : 22 Sample Multiplier: 1

Instrument :
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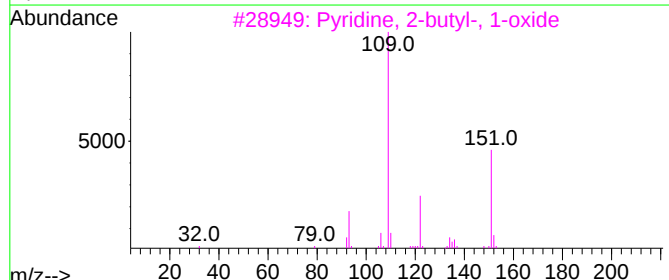
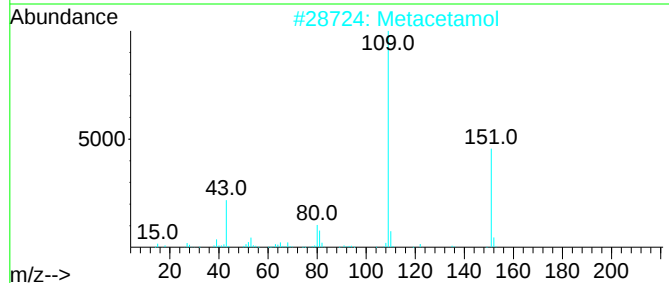
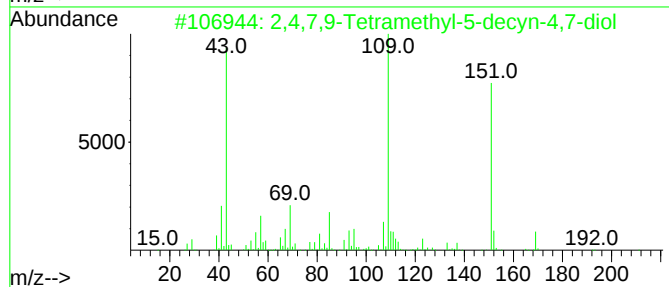
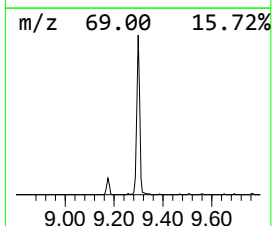
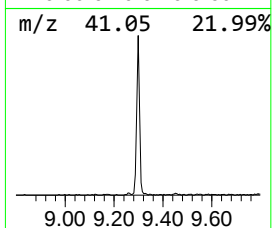
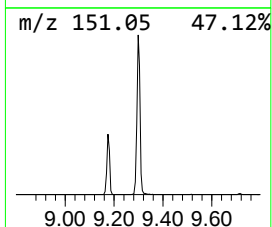
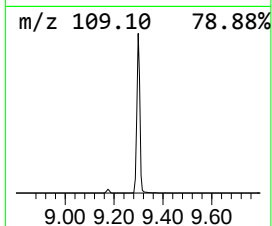
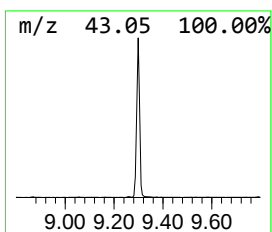
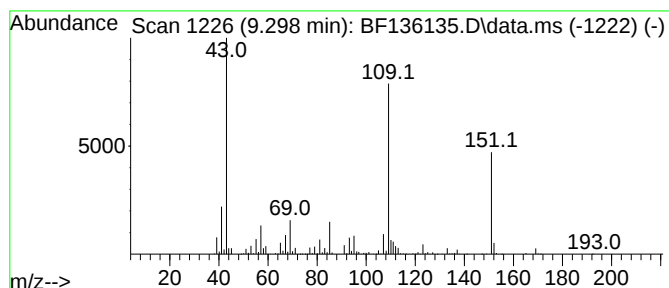
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.298	26.06 ng	823750	Acenaphthene-d10	9.857

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91	
2	Metacetamol	151	C8H9NO2	000621-42-1	64	
3	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59	
4	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	59	
5	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3	1000107-08-7	45	



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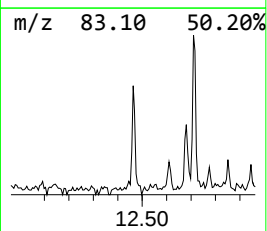
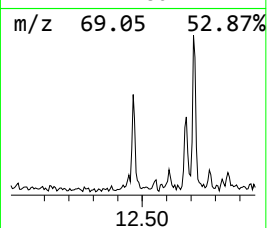
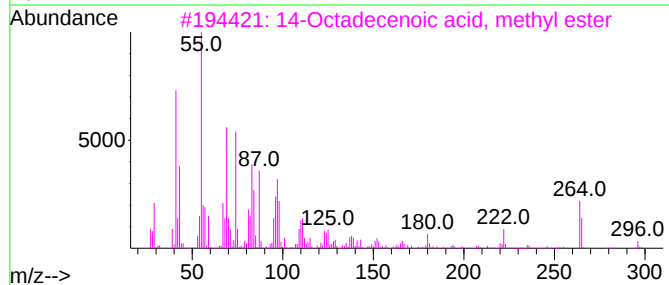
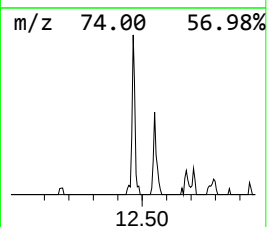
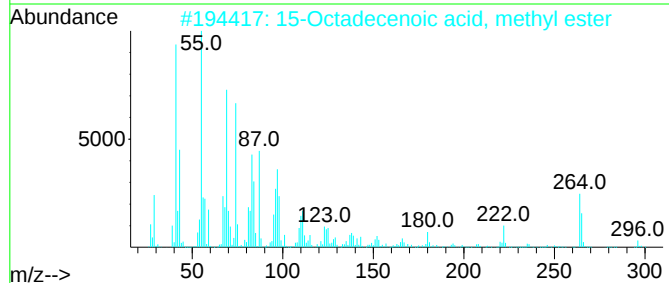
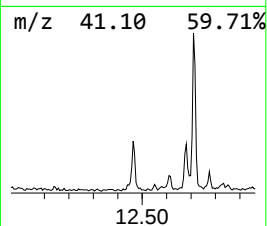
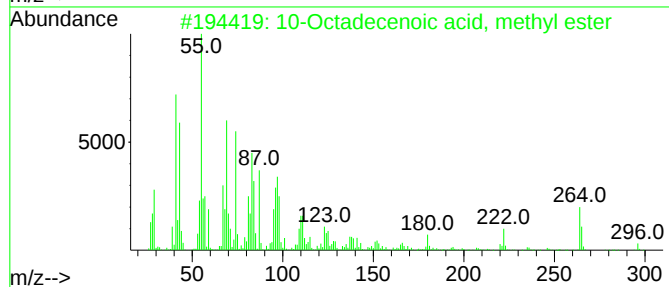
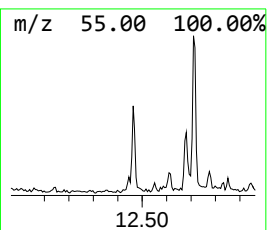
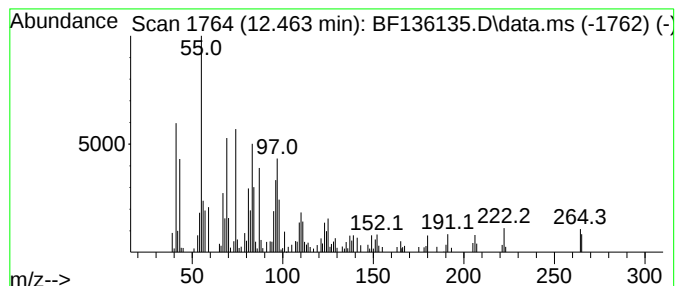
Instrument :
BNA_F
ClientSampleId :
ETGI-293

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 10-Octadecenoic acid, methyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.463	3.03 ng	86433	Phenanthrene-d10	11.345	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94
2	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	91
3	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
4	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91
5	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	90



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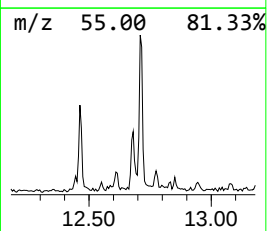
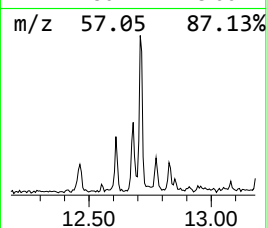
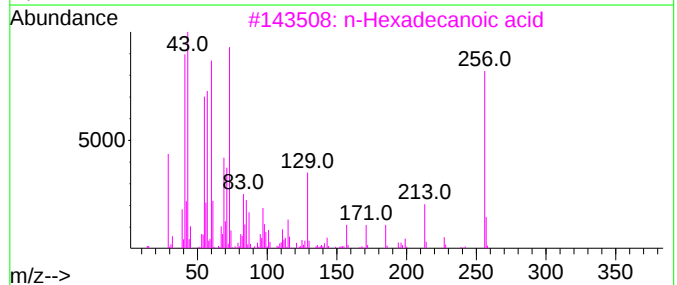
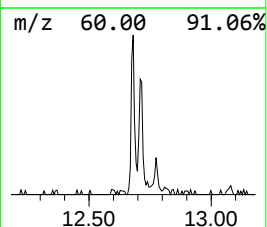
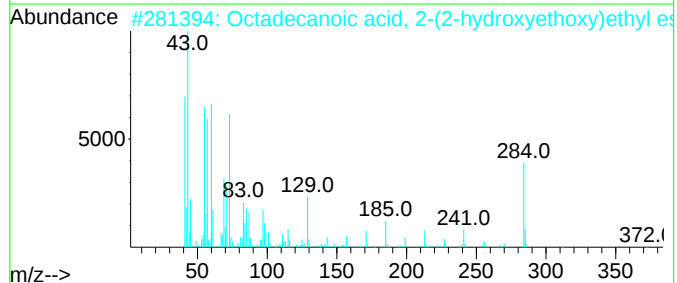
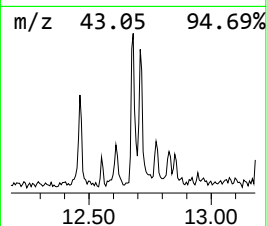
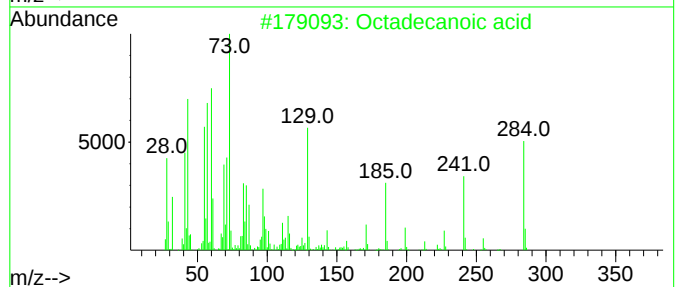
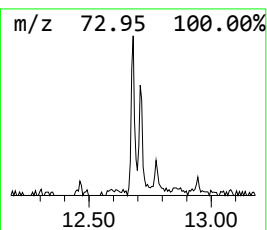
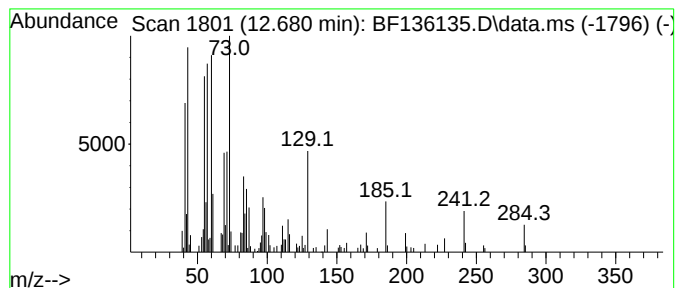
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.680	2.94 ng	105222	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	68



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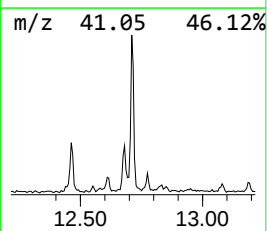
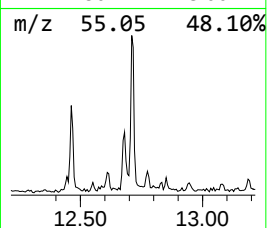
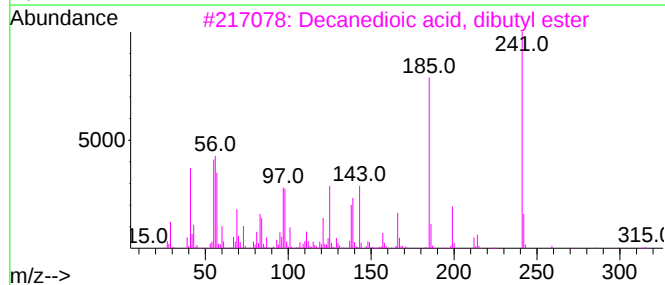
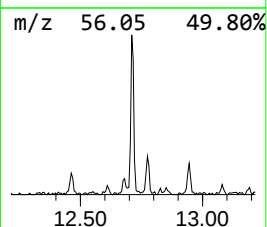
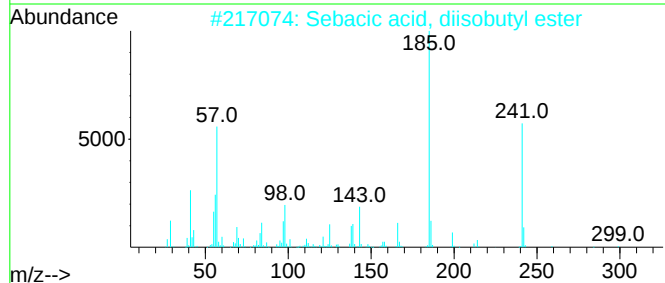
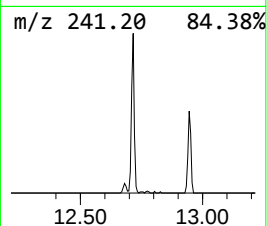
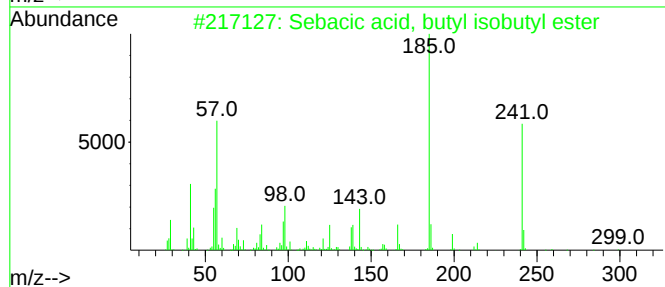
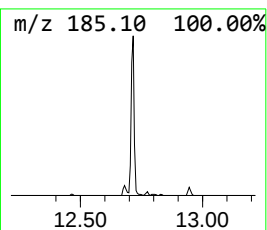
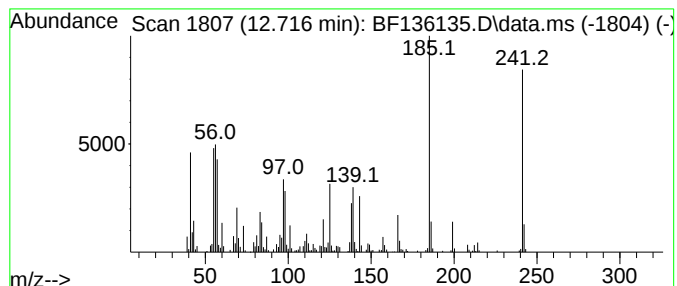
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Sebaccic acid, butyl isobuty... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	7.89 ng	282072	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sebaccic acid, butyl isobutyl ester	314	C18H34O4	1000354-21-5	74
2			Sebaccic acid, diisobutyl ester	314	C18H34O4	1000354-21-4	72
3			Decanedioic acid, dibutyl ester	314	C18H34O4	000109-43-3	58
4			Sebaccic acid, butyl 2-ethylhexyl...	370	C22H42O4	1000354-19-9	50
5			Sebaccic acid, butyl 3-hexyl ester	342	C20H38O4	1000355-53-9	47



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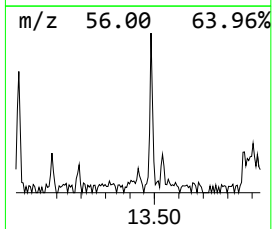
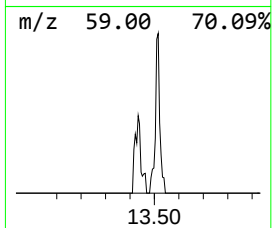
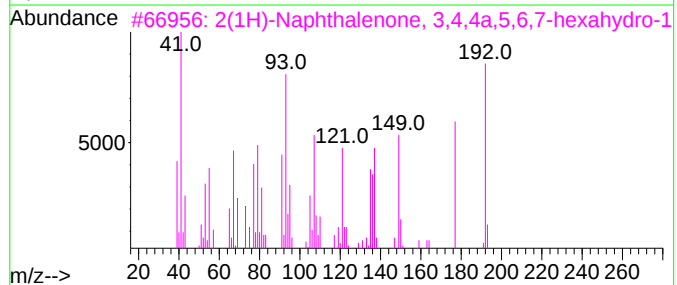
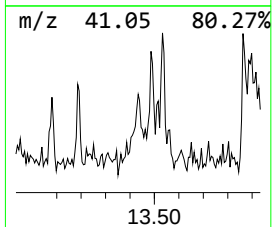
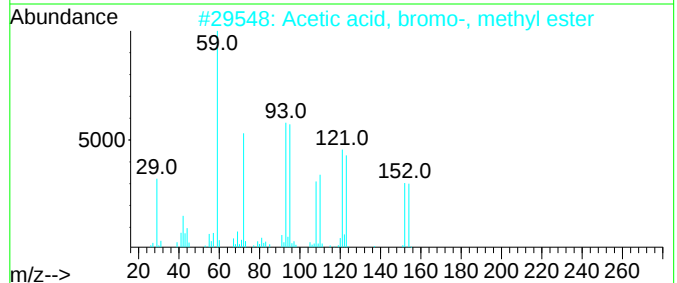
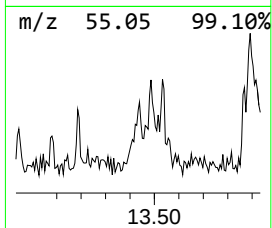
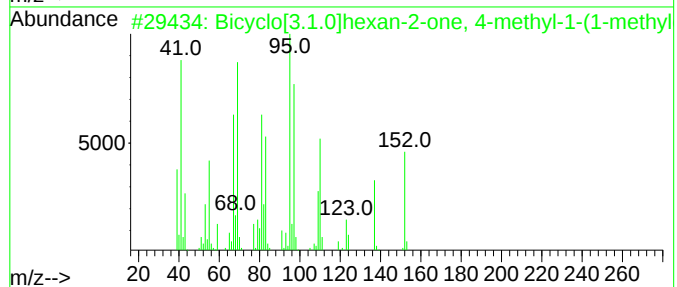
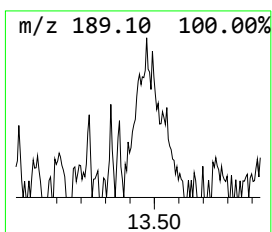
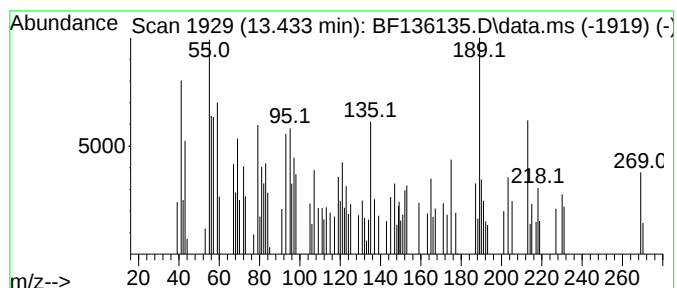
Instrument :
BNA_F
ClientSampleId :
ETGI-293

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Bicyclo[3.1.0]hexan-2-one, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.433	2.03 ng	72612	Chrysene-d12	14.004	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.0]hexan-2-one, 4-met...	152	C10H16O	002506-61-8	56
2	Acetic acid, bromo-, methyl ester	152	C3H5BrO2	000096-32-2	25
3	2(1H)-Naphthalenone, 3,4,4a,5,6,...	192	C13H20O	004668-61-5	15
4	cis-11,12-Epoxytetradecen-1-ol	270	C16H30O3	1000130-82-5	15
5	9H-Purine-9-ethanol, 6-amino-.al...	193	C8H11N5O	000712-00-5	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110323\
Data File : BF136135.D
Acq On : 03 Nov 2023 20:42
Operator : CG\JU
Sample : 05213-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-293

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2,4,7,9-Tetrame...	9.298	26.1	ng	823750	3	9.857	632269	20.0
10-Octadecenoic...	12.463	3.0	ng	86433	4	11.345	569840	20.0
Octadecanoic acid	12.680	2.9	ng	105222	5	14.004	714594	20.0
Sebacic acid, b...	12.716	7.9	ng	282072	5	14.004	714594	20.0
Bicyclo[3.1.0]h...	13.433	2.0	ng	72612	5	14.004	714594	20.0