

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082018\
 Data File : BF108311.D
 Acq On : 21 Aug 2018 00:49
 Operator : JU/SJ
 Sample : J4497-01
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CARLSTADT-FRONT

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

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-BF080818.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.396	4	10	21	rVB	332734	488096	14.15%	1.593%
2	5.272	494	499	508	rVB	128365	153995	4.46%	0.502%
3	5.649	558	563	567	rBV	3068521	3209859	93.04%	10.474%
4	6.643	726	732	735	rBV	3330834	3353190	97.19%	10.942%
5	6.790	752	757	760	rBV	3615765	3282187	95.13%	10.710%
6	7.019	792	796	799	rBV	1143592	931967	27.01%	3.041%
7	7.178	818	823	826	rBV	2824966	2605555	75.52%	8.502%
8	7.578	886	891	895	rBV	2011758	2023807	58.66%	6.604%
9	8.301	1010	1014	1030	rVB	1278653	1082669	31.38%	3.533%
10	9.372	1191	1196	1200	rBV	3543472	3450032	100.00%	11.258%
11	9.766	1259	1263	1269	rBV	183197	169244	4.91%	0.552%
12	10.066	1309	1314	1318	rBV	1092788	1030313	29.86%	3.362%
13	10.854	1444	1448	1461	rBV	1773945	1777822	51.53%	5.801%
14	11.560	1564	1568	1571	rBV	1158195	1024523	29.70%	3.343%
15	11.583	1571	1572	1575	rVV	197231	112666	3.27%	0.368%
16	11.636	1575	1581	1584	rVV	52120	44802	1.30%	0.146%
17	12.089	1655	1658	1662	rVB2	40615	37997	1.10%	0.124%
18	12.177	1669	1673	1675	rBV2	48368	52842	1.53%	0.172%
19	12.619	1744	1748	1752	rBV3	31513	63162	1.83%	0.206%
20	12.701	1759	1762	1767	rBV4	26278	35009	1.01%	0.114%
21	12.777	1772	1775	1779	rBV	353736	320694	9.30%	1.046%
22	13.013	1812	1815	1820	rVB	308362	287130	8.32%	0.937%
23	13.148	1833	1838	1841	rBV	3317690	2869575	83.18%	9.364%
24	13.230	1848	1852	1856	rBV4	21624	37934	1.10%	0.124%
25	13.336	1868	1870	1876	rVB2	31821	43290	1.25%	0.141%
26	14.042	1987	1990	2001	rVB4	110527	217415	6.30%	0.709%
27	14.213	2015	2019	2022	rBV2	788351	872164	25.28%	2.846%
28	14.242	2022	2024	2031	rVB	128215	116579	3.38%	0.380%
29	15.066	2161	2164	2172	rVB	171486	190839	5.53%	0.623%
30	15.307	2202	2205	2208	rBV	95114	133792	3.88%	0.437%
31	15.713	2271	2274	2279	rVB	74968	96434	2.80%	0.315%
32	15.783	2281	2286	2290	rVB	389241	530805	15.39%	1.732%

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Instrument :
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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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

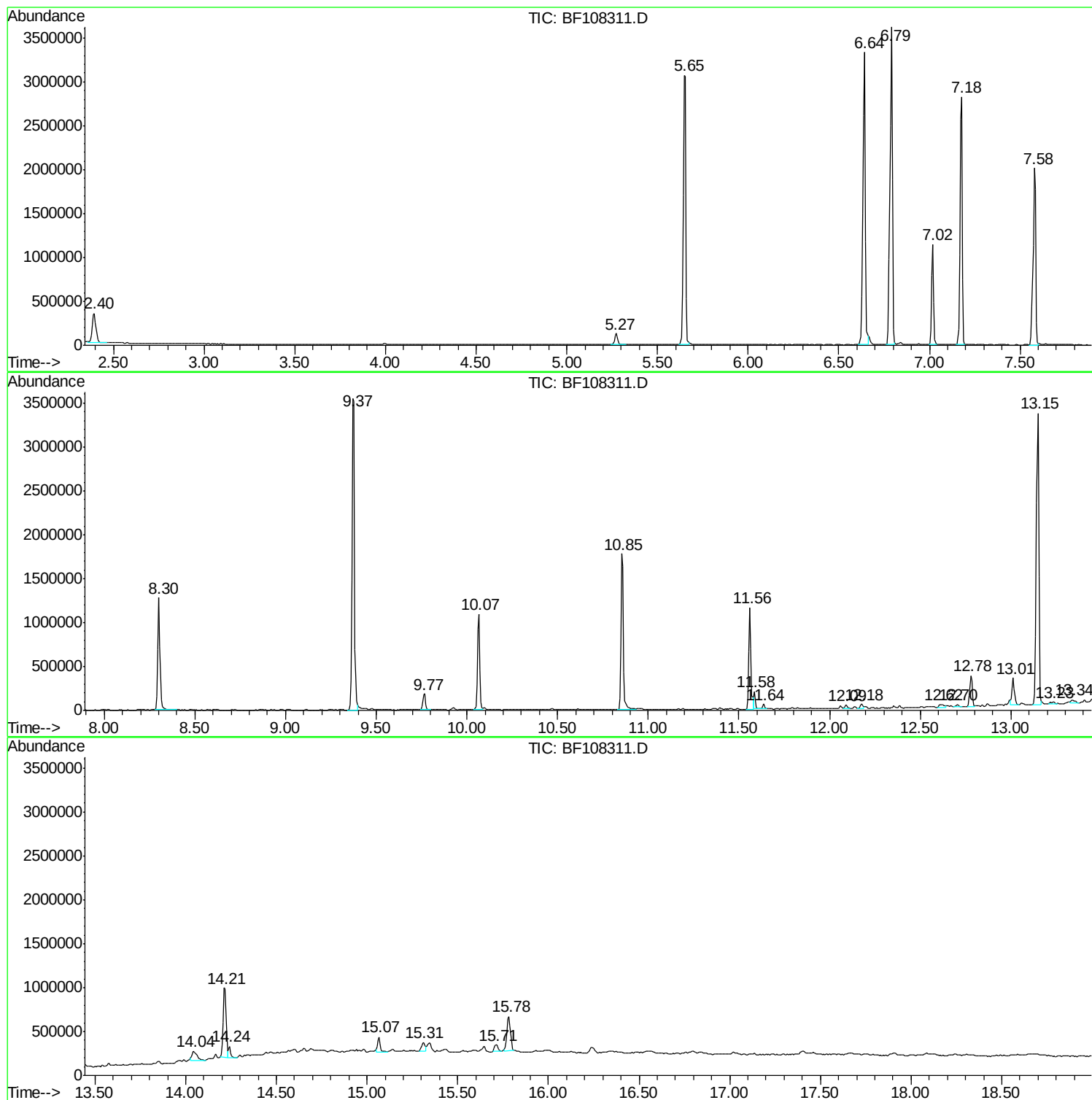
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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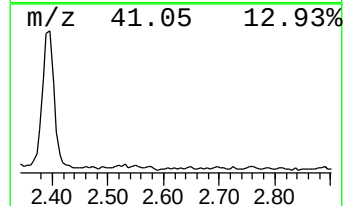
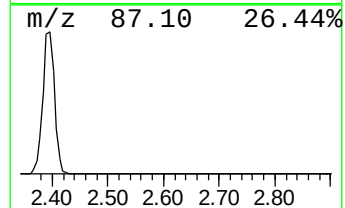
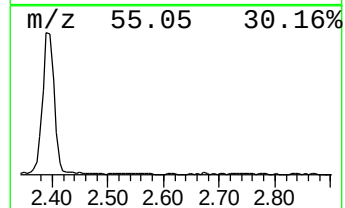
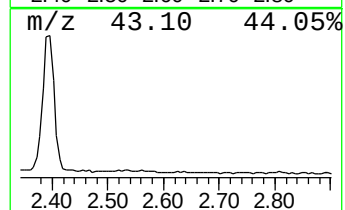
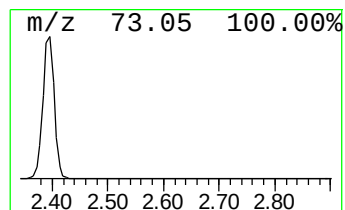
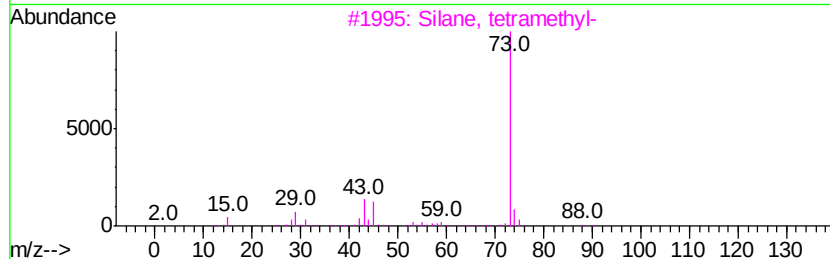
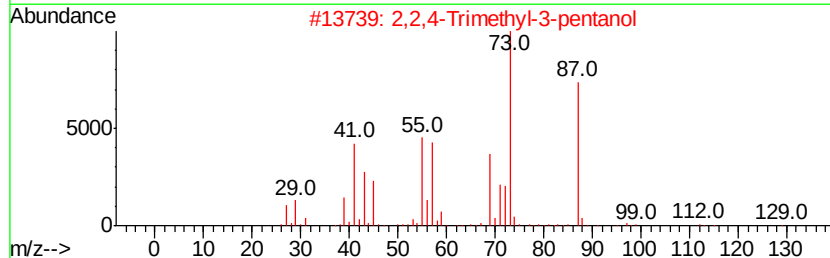
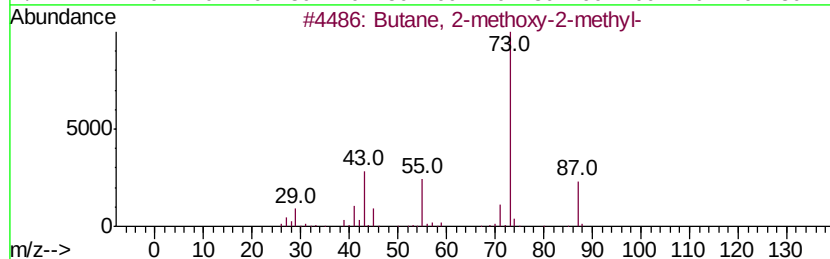
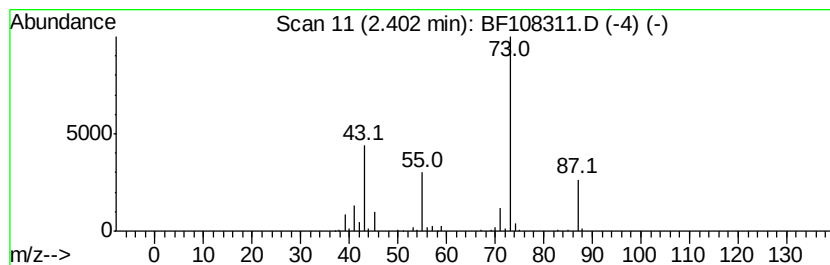
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.40	10.47 ng	488096	1,4-Dichlorobenzene-d4	7.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25



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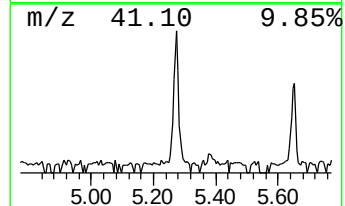
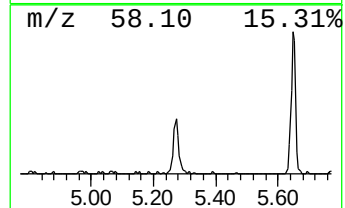
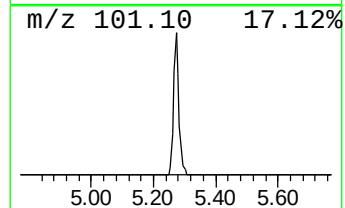
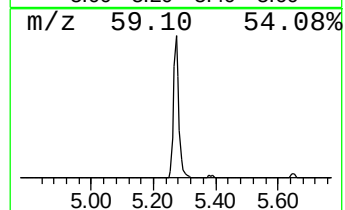
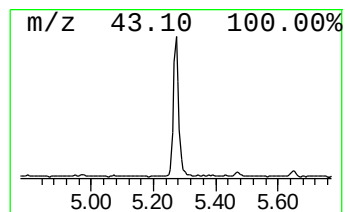
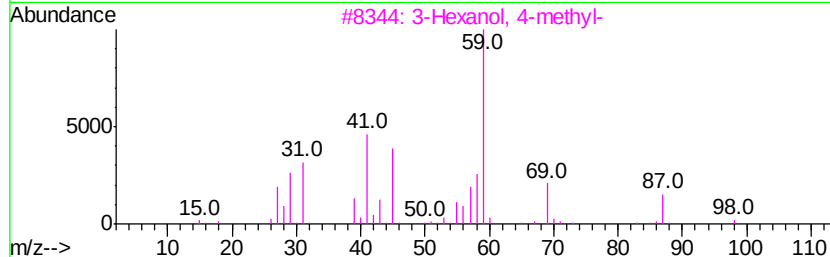
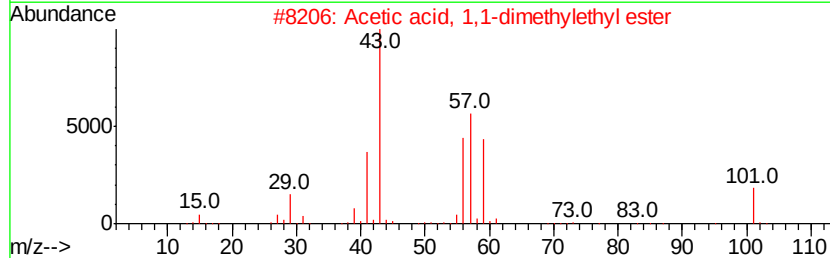
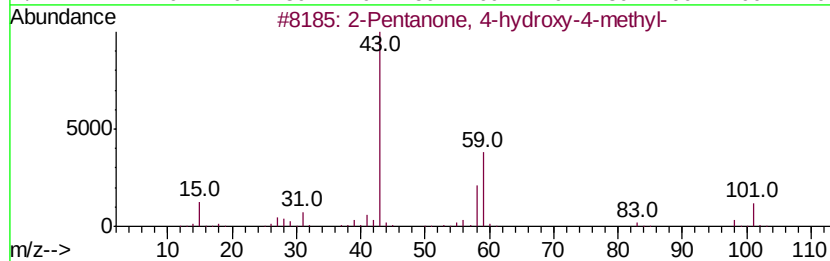
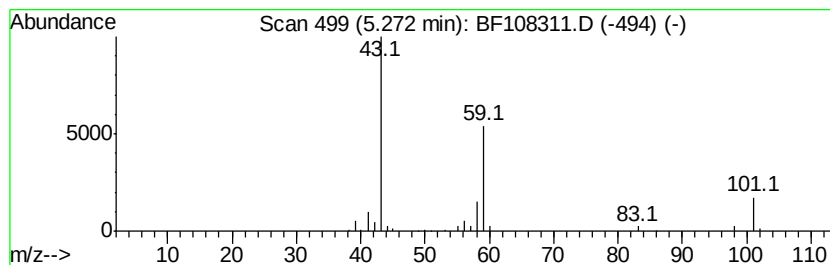
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.27	3.30 ng	153995	1,4-Dichlorobenzene-d4	7.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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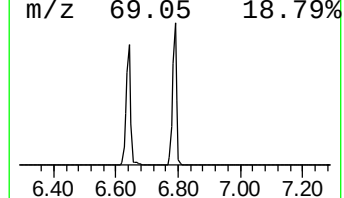
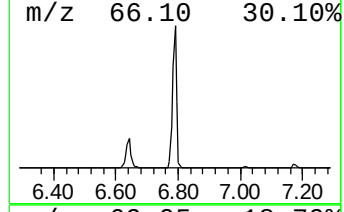
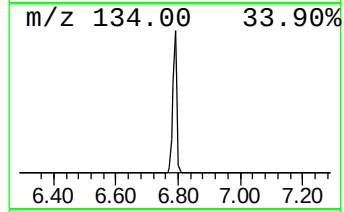
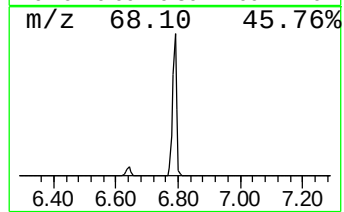
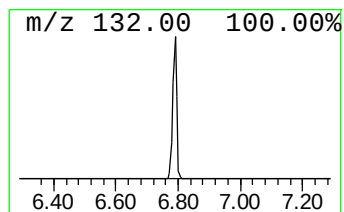
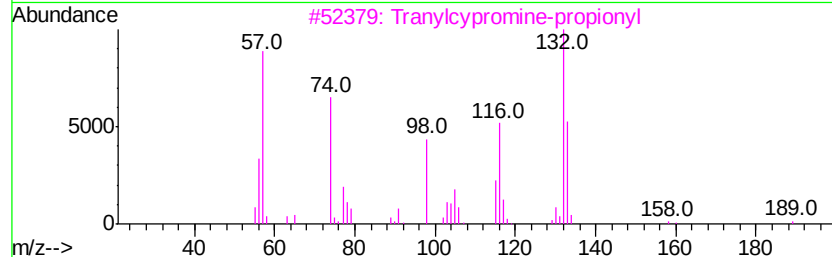
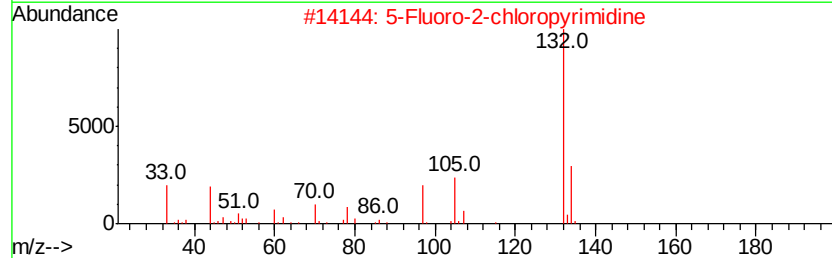
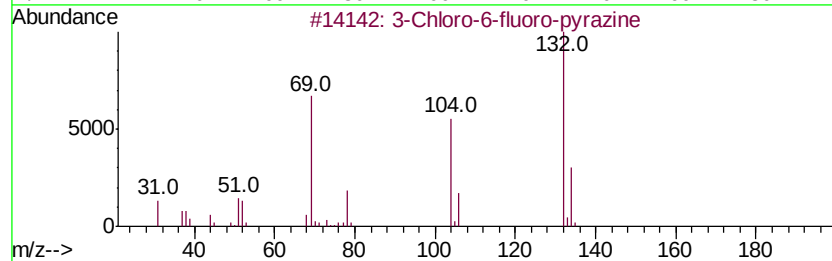
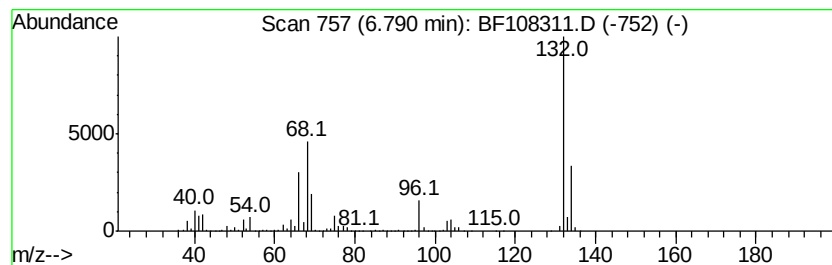
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.79 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.79	70.44 ng	3282190	1,4-Dichlorobenzene-d4	7.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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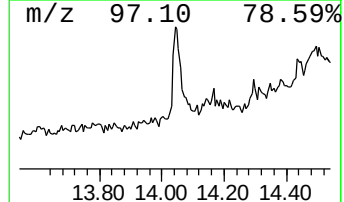
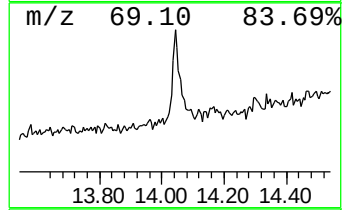
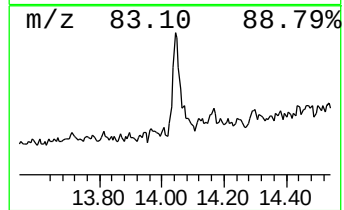
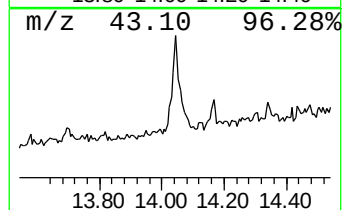
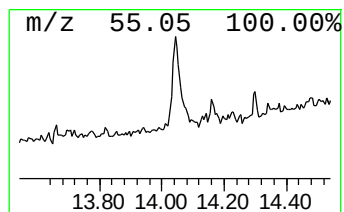
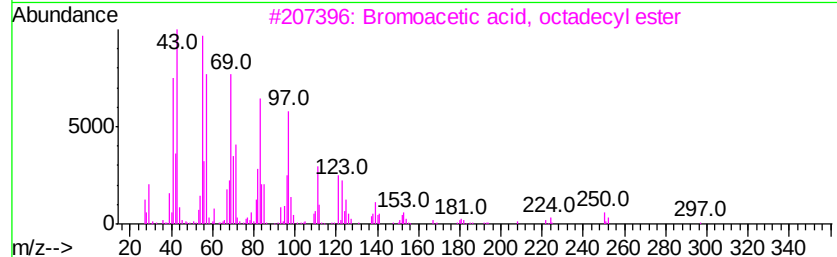
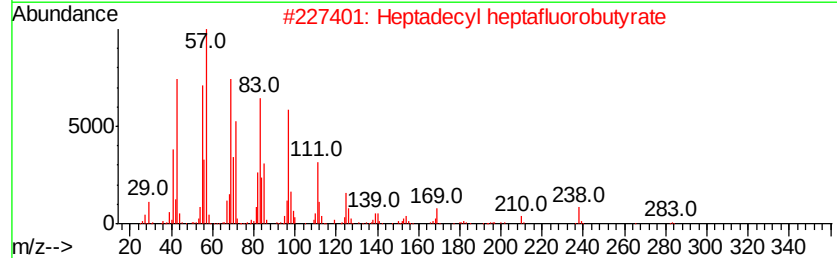
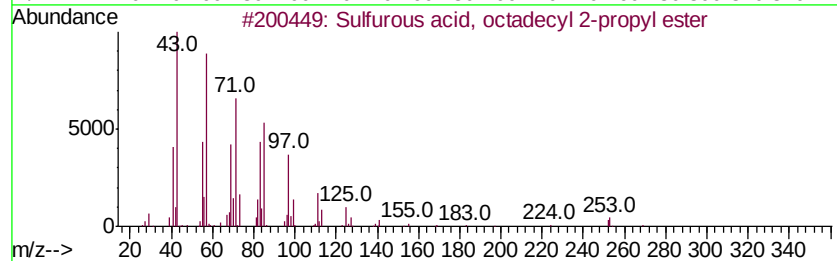
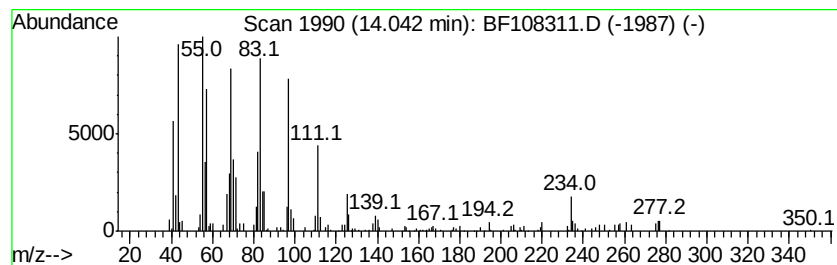
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Sulfurous acid, octadecyl 2... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	4.99 ng	217415	Chrysene-d12	14.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	80
2		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	72
3		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	72
4		Acetic acid n-octadecyl ester	312	C20H40O2	000822-23-1	58
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	53



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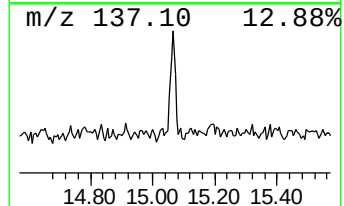
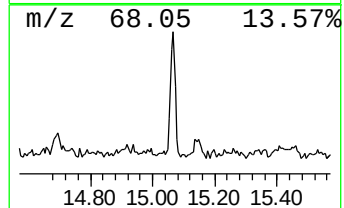
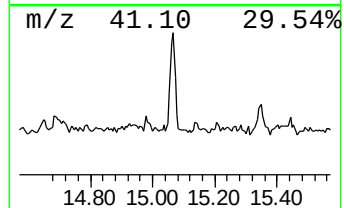
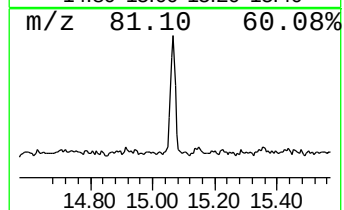
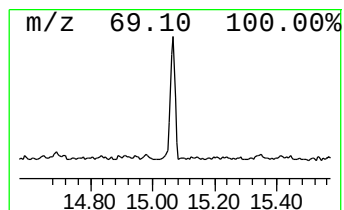
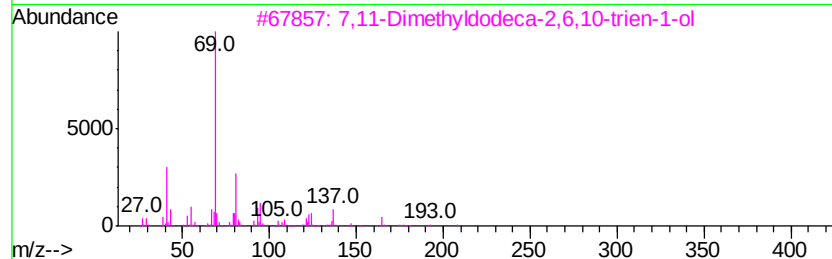
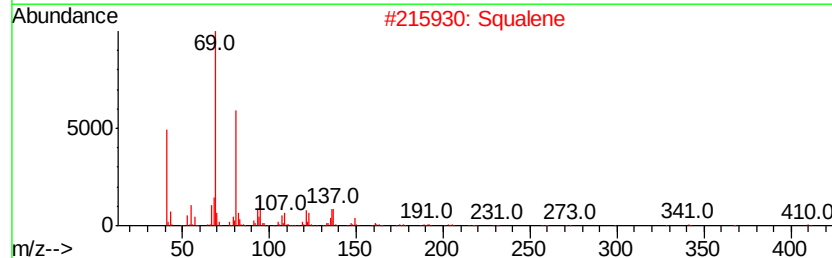
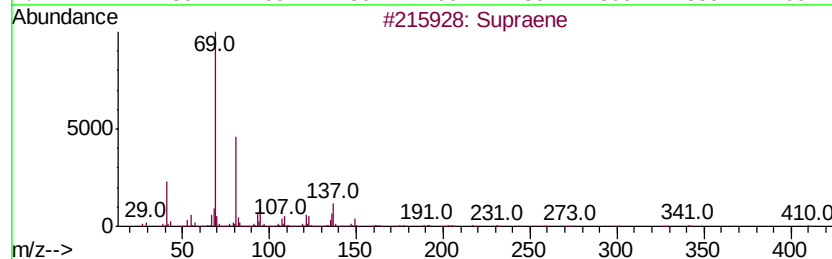
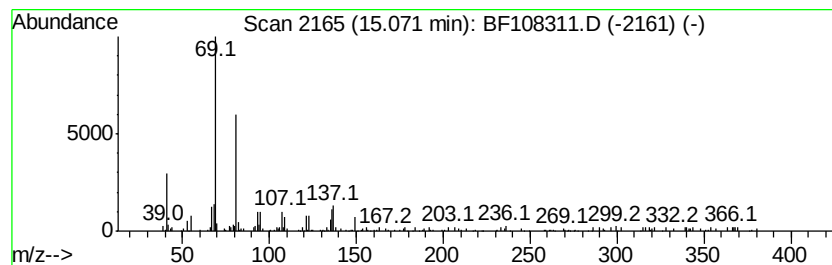
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	7.19 ng	190839	Perylene-d12	15.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	91
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	81
4		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	81
5		3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	72



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ClientSampleId :
CARLSTADT-FRONT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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-methoxy...	2.40	10.5	ng	488096	1	7.02	931967	20.0
2-Pentanone, 4-hy...	5.27	3.3	ng	153995	1	7.02	931967	20.0
unknown6.79	6.79	70.4	ng	3282190	1	7.02	931967	20.0
Sulfurous acid, o...	14.04	5.0	ng	217415	5	14.22	872164	20.0
Supraene	15.07	7.2	ng	190839	6	15.78	530805	20.0