

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062218\
 Data File : BF106753.D
 Acq On : 23 Jun 2018 11:42
 Operator : JU/SJ
 Sample : J3597-04
 Misc :
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W-21

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-BF061918.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	5.190	482	485	495	rBB	28591	31072	2.55%	0.378%
2	5.601	551	555	562	rBV	575833	509213	41.85%	6.187%
3	6.601	721	725	731	rBV	337864	320949	26.38%	3.899%
4	6.737	744	748	751	rBV	1000562	856823	70.42%	10.410%
5	6.960	782	786	789	rBV	301848	250404	20.58%	3.042%
6	7.113	808	812	816	rBV	877030	832753	68.44%	10.118%
7	7.525	877	882	885	rBV	692015	642631	52.82%	7.808%
8	7.601	892	895	902	rVB3	12936	14775	1.21%	0.180%
9	8.242	1000	1004	1007	rBV	316131	267600	21.99%	3.251%
10	8.795	1096	1098	1103	rVB	24582	18795	1.54%	0.228%
11	8.966	1120	1127	1131	rBV2	26519	29316	2.41%	0.356%
12	9.148	1151	1158	1159	rBV3	12285	14649	1.20%	0.178%
13	9.213	1166	1169	1174	rBV4	9408	14939	1.23%	0.182%
14	9.313	1182	1186	1190	rBV	1155325	1063035	87.37%	12.915%
15	9.707	1250	1253	1258	rVB	40426	37283	3.06%	0.453%
16	10.001	1299	1303	1308	rVB	303381	264012	21.70%	3.208%
17	10.407	1370	1372	1375	rVB	20202	15191	1.25%	0.185%
18	10.648	1411	1413	1416	rVB	21076	16929	1.39%	0.206%
19	10.795	1434	1438	1441	rBV	687976	627480	51.57%	7.624%
20	10.883	1450	1453	1457	rVB	14899	12922	1.06%	0.157%
21	11.489	1553	1556	1560	rBV	304206	279451	22.97%	3.395%
22	12.877	1789	1792	1797	rVB2	33048	29586	2.43%	0.359%
23	12.960	1803	1806	1810	rVB2	17751	17008	1.40%	0.207%
24	13.077	1822	1826	1829	rBV	1316770	1216730	100.00%	14.783%
25	13.583	1909	1912	1915	rVB	24629	18136	1.49%	0.220%
26	13.624	1915	1919	1922	rBV2	17096	15370	1.26%	0.187%
27	13.954	1972	1975	1980	rBV2	42449	44544	3.66%	0.541%
28	14.148	2004	2008	2011	rBV	379094	344605	28.32%	4.187%
29	14.283	2028	2031	2034	rVB3	15895	14223	1.17%	0.173%
30	14.601	2082	2085	2090	rBV2	25209	27235	2.24%	0.331%
31	14.918	2136	2139	2142	rVB	32747	30192	2.48%	0.367%
32	15.277	2196	2200	2203	rVB	31195	35082	2.88%	0.426%
33	15.689	2264	2270	2275	rBV	197674	269014	22.11%	3.268%
34	16.136	2342	2346	2352	rVB3	21506	31624	2.60%	0.384%

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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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35	16.677	2434	2438	2443	rVB5	10397	17139	1.41%	0.208%
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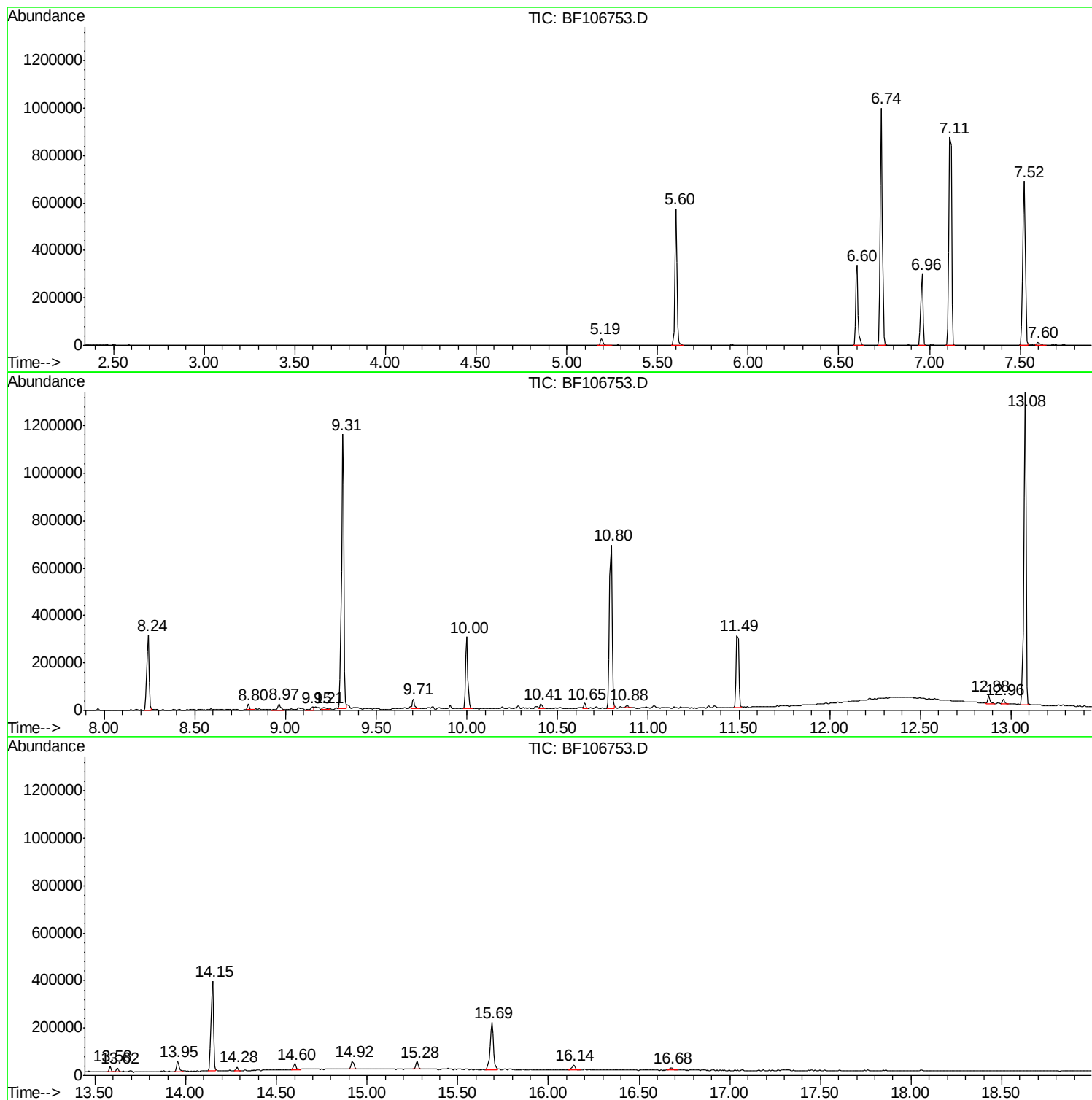
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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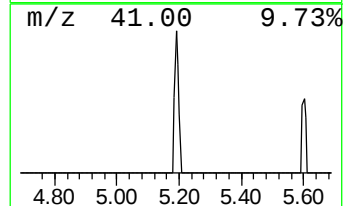
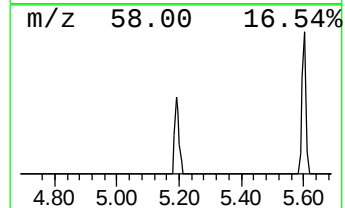
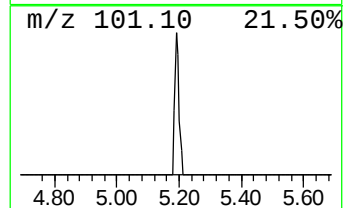
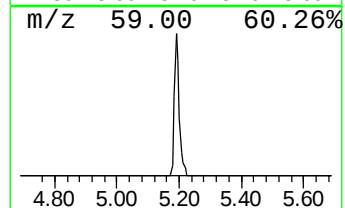
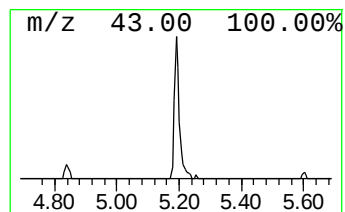
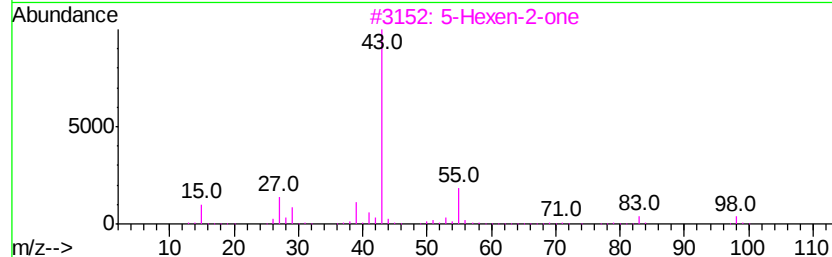
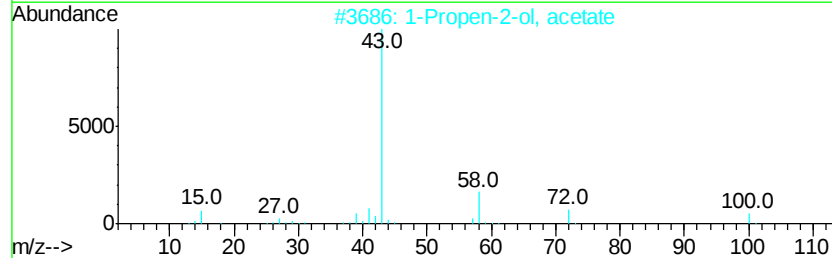
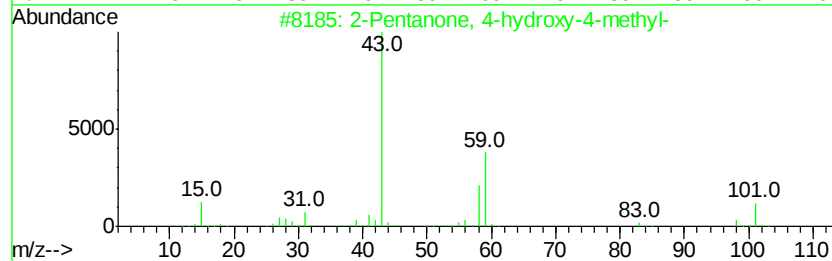
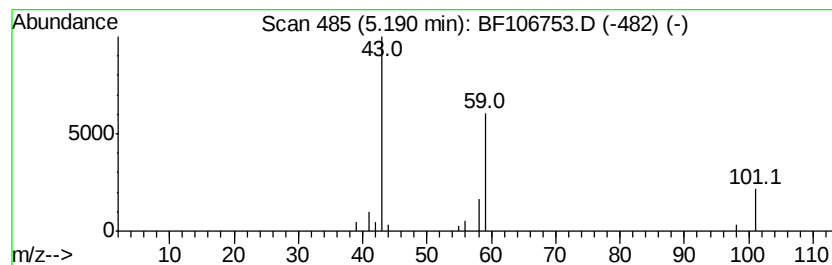
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	2.48 ng	31072	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
3		5-Hexen-2-one	98	C6H10O	000109-49-9	7
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	7
5		Guanidine	59	CH5N3	000113-00-8	5



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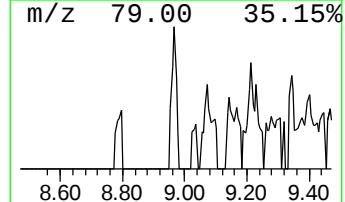
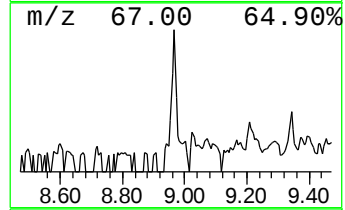
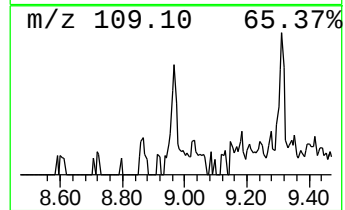
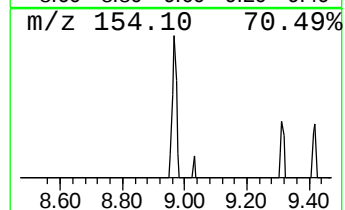
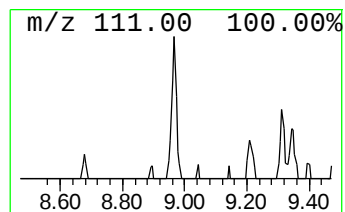
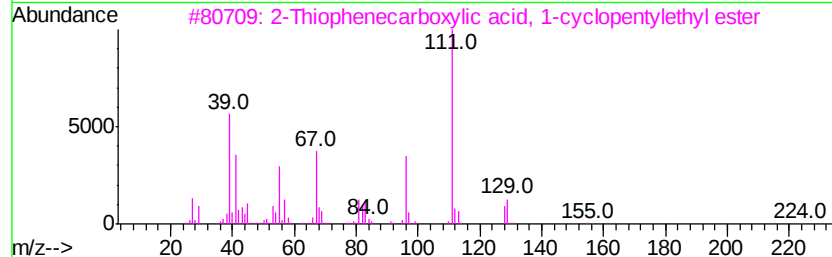
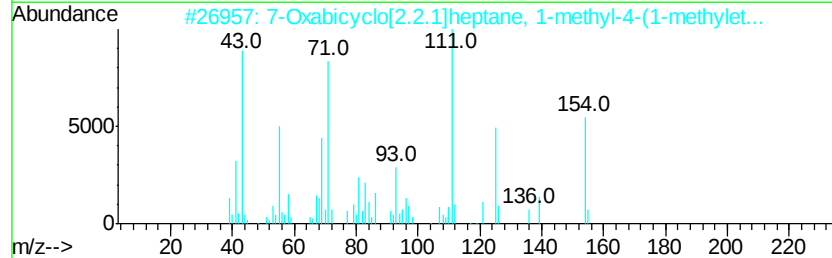
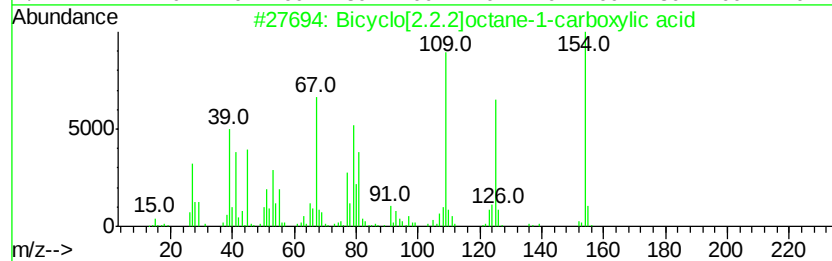
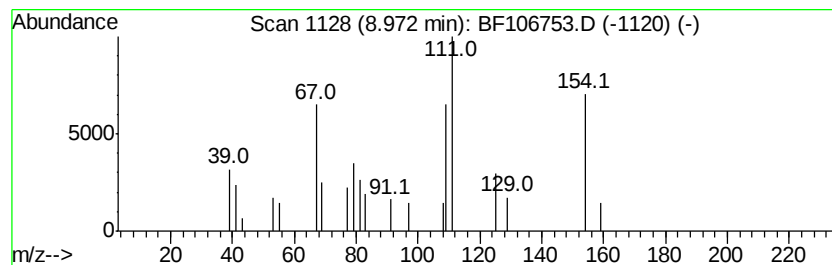
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown8.97 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.97	2.19 ng	29316	Naphthalene-d8	8.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[2.2.2]octane-1-carboxylic acid	154	C9H14O2	000699-55-8	42
2		7-Oxabicyclo[2.2.1]heptane, 1-methyl-4-(1-methylethyl)-	154	C10H18O	000470-67-7	38
3		2-Thiophenecarboxylic acid, 1-cyclopentylethyl ester	224	C12H16O2S	1000278-88-4	27
4		3,4-Dimethyl-3-pyrrolin-2-one	111	C6H9NO	004030-22-2	22
5		1-Cyclooctene-1-carboxylic acid	154	C9H14O2	004103-09-7	22



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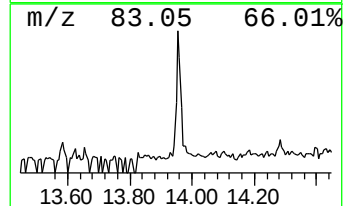
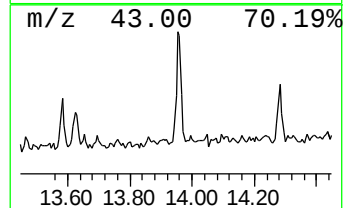
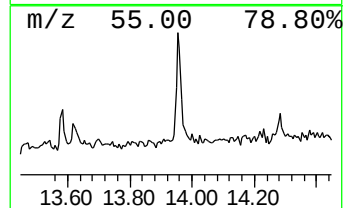
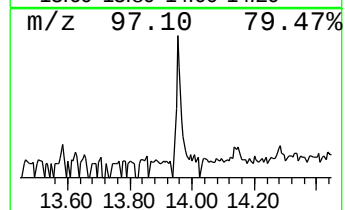
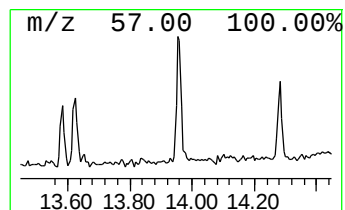
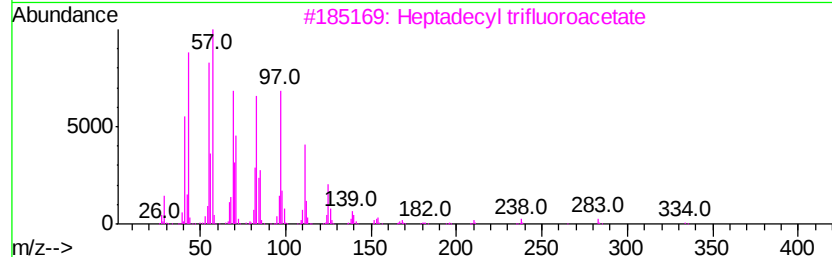
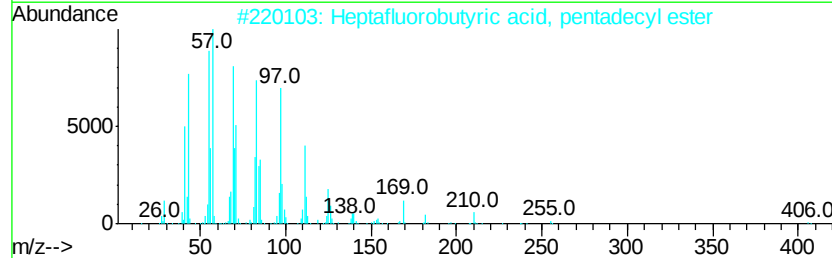
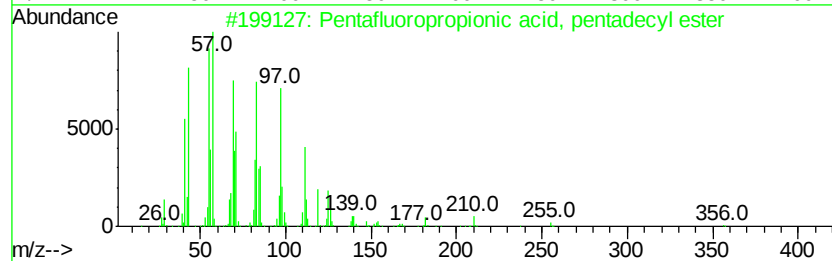
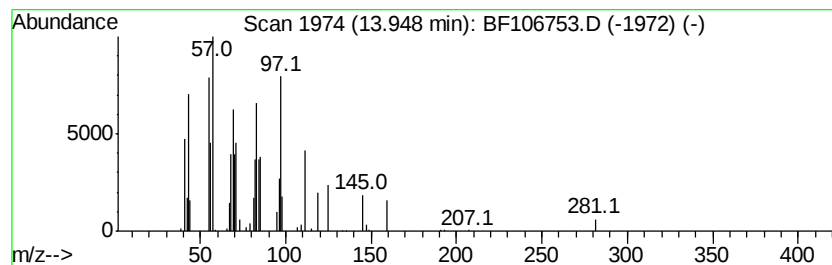
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	2.59 ng	44544	Chrysene-d12	14.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
2		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
3		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
4		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
5		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91



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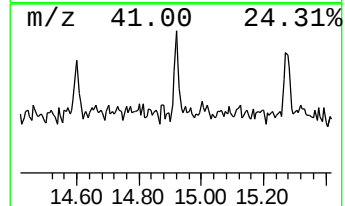
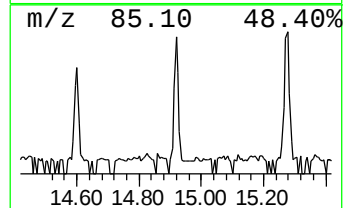
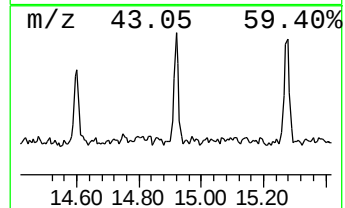
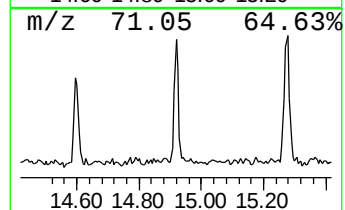
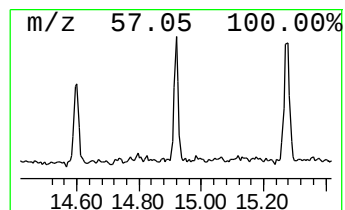
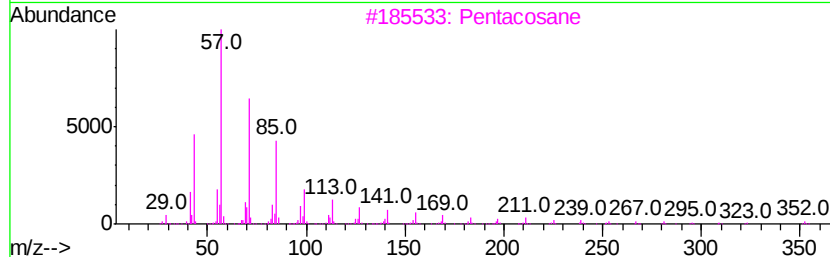
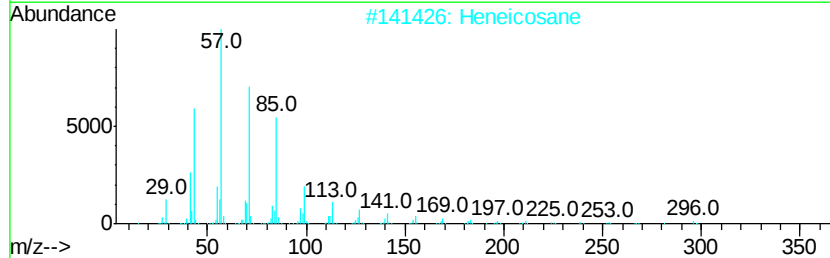
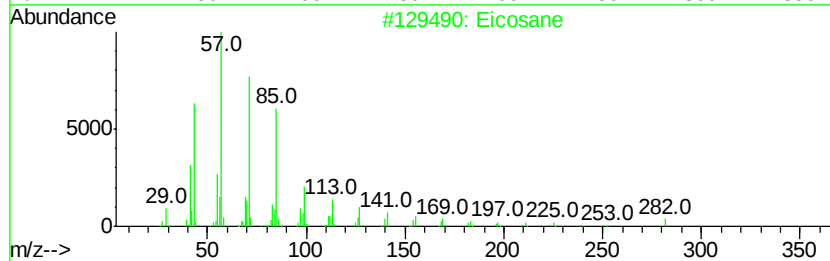
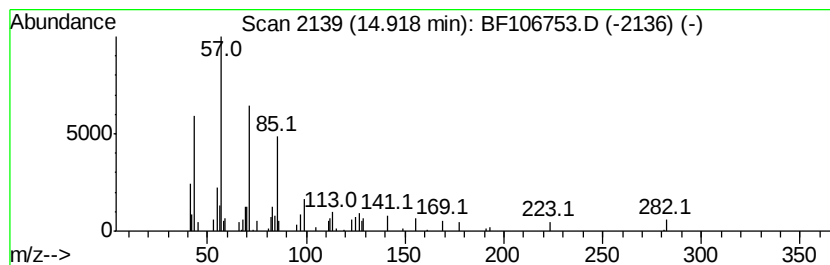
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	2.24 ng	30192	Perylene-d12	15.69

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	97
2	Heneicosane		296	C21H44	000629-94-7	87
3	Pentacosane		352	C25H52	000629-99-2	87
4	Octacosane		394	C28H58	000630-02-4	87
5	Octadecane		254	C18H38	000593-45-3	87



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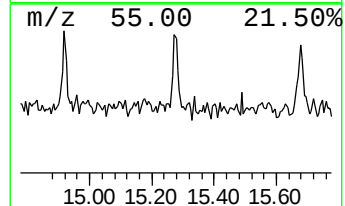
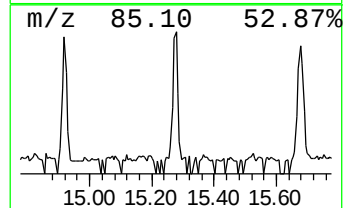
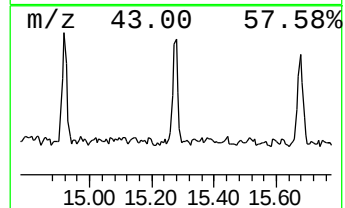
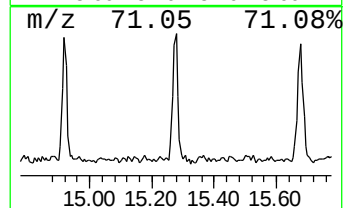
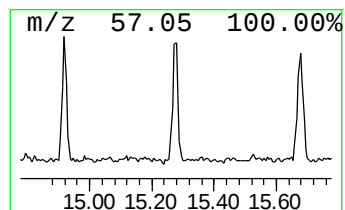
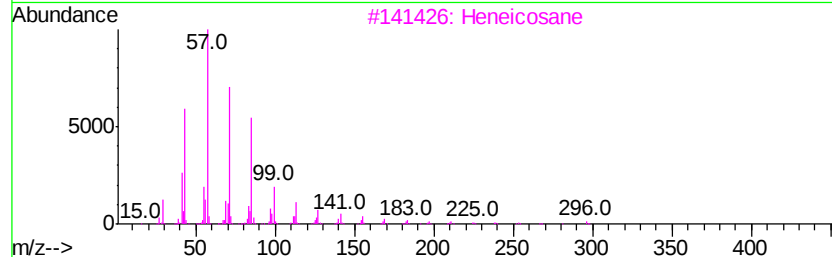
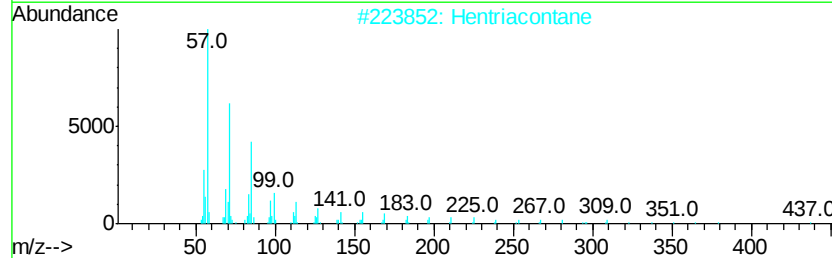
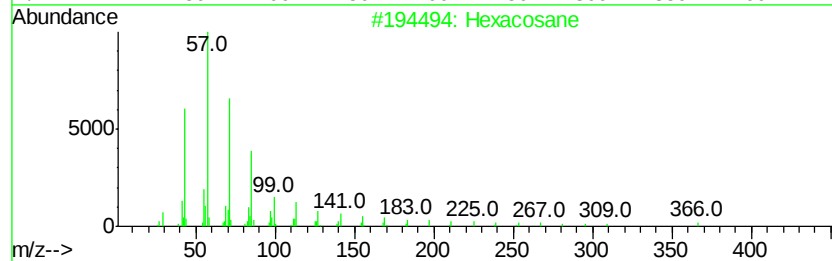
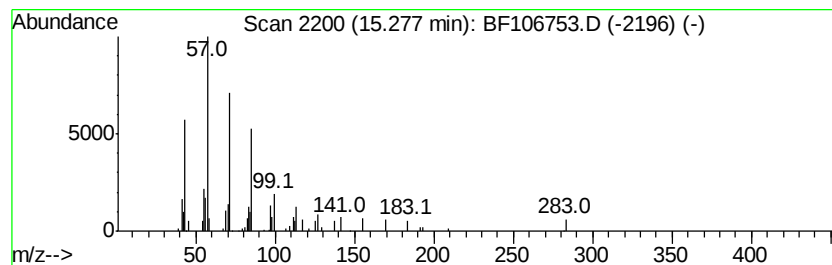
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.28	2.61 ng	35082	Perylene-d12	15.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Hentriacontane	437	C31H64	000630-04-6	91
3		Heneicosane	296	C21H44	000629-94-7	90
4		Octacosane	394	C28H58	000630-02-4	90
5		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90



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ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-21

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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
2-Pentanone, 4-hy...	5.19	2.5	ng	31072	1	6.96	250404	20.0
unknown8.97	8.97	2.2	ng	29316	2	8.24	267600	20.0
Pentafluoropropio...	13.95	2.6	ng	44544	5	14.15	344605	20.0
Eicosane	14.92	2.2	ng	30192	6	15.69	269014	20.0
Hexacosane	15.28	2.6	ng	35082	6	15.69	269014	20.0