

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081719\
 Data File : BF116358.D
 Acq On : 17 Aug 2019 15:38
 Operator : HP/JU
 Sample : K4391-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 E-CORNER

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-BF073019.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	3.881	301	305	321	rVB	151450	252231	8.19%	0.878%
2	4.463	399	404	411	rVB2	23977	33844	1.10%	0.118%
3	5.022	495	499	503	rBV2	30636	38511	1.25%	0.134%
4	5.228	530	534	537	rBV	29529	32485	1.06%	0.113%
5	5.439	567	570	591	rBV	2201440	2552530	82.90%	8.888%
6	5.834	631	637	641	rVB2	23044	34708	1.13%	0.121%
7	5.963	654	659	664	rVB3	32905	38230	1.24%	0.133%
8	6.057	672	675	682	rVB3	37710	47659	1.55%	0.166%
9	6.451	738	742	755	rBV	2633325	2784711	90.44%	9.696%
10	6.581	761	764	772	rVB	2867502	2702341	87.76%	9.410%
11	6.810	800	803	815	rVB	962181	891608	28.96%	3.105%
12	6.963	826	829	840	rBV	2369833	2174179	70.61%	7.570%
13	7.375	895	899	919	rBV	1767034	1785819	58.00%	6.218%
14	8.086	1017	1020	1029	rBV	1126029	1114251	36.19%	3.880%
15	9.157	1199	1202	1214	rBV	3076688	3079130	100.00%	10.721%
16	9.275	1219	1222	1226	rVB	44724	45798	1.49%	0.159%
17	9.557	1267	1270	1278	rBV	286413	260588	8.46%	0.907%
18	9.839	1315	1318	1327	rVB	1613555	1335828	43.38%	4.651%
19	10.627	1449	1452	1465	rBV	1692975	1873989	60.86%	6.525%
20	11.327	1567	1571	1580	rBV	1415599	1338899	43.48%	4.662%
21	11.392	1580	1582	1586	rVB2	59369	51915	1.69%	0.181%
22	11.851	1656	1660	1672	rBV2	122452	183808	5.97%	0.640%
23	12.368	1745	1748	1752	rBV2	47054	81086	2.63%	0.282%
24	12.904	1835	1839	1842	rBV	3309903	2929579	95.14%	10.201%
25	13.127	1872	1877	1886	rBV	35300	53815	1.75%	0.187%
26	13.792	1986	1990	2011	rBV3	249100	530620	17.23%	1.848%
27	13.968	2017	2020	2032	rVB	1068811	1054132	34.23%	3.670%
28	14.415	2092	2096	2098	rBV	34860	34562	1.12%	0.120%
29	14.709	2141	2146	2151	rBV	40213	42985	1.40%	0.150%
30	14.786	2155	2159	2163	rBV	283614	262481	8.52%	0.914%
31	15.039	2197	2202	2206	rBV	47384	52943	1.72%	0.184%
32	15.421	2260	2267	2286	rBV	582125	933653	30.32%	3.251%
33	15.821	2329	2335	2340	rBV	38211	54579	1.77%	0.190%
34	16.304	2412	2417	2421	rBV2	21585	35713	1.16%	0.124%

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Misc :
ALS Vial : 12 Sample Multiplier: 1

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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-BF073019.M
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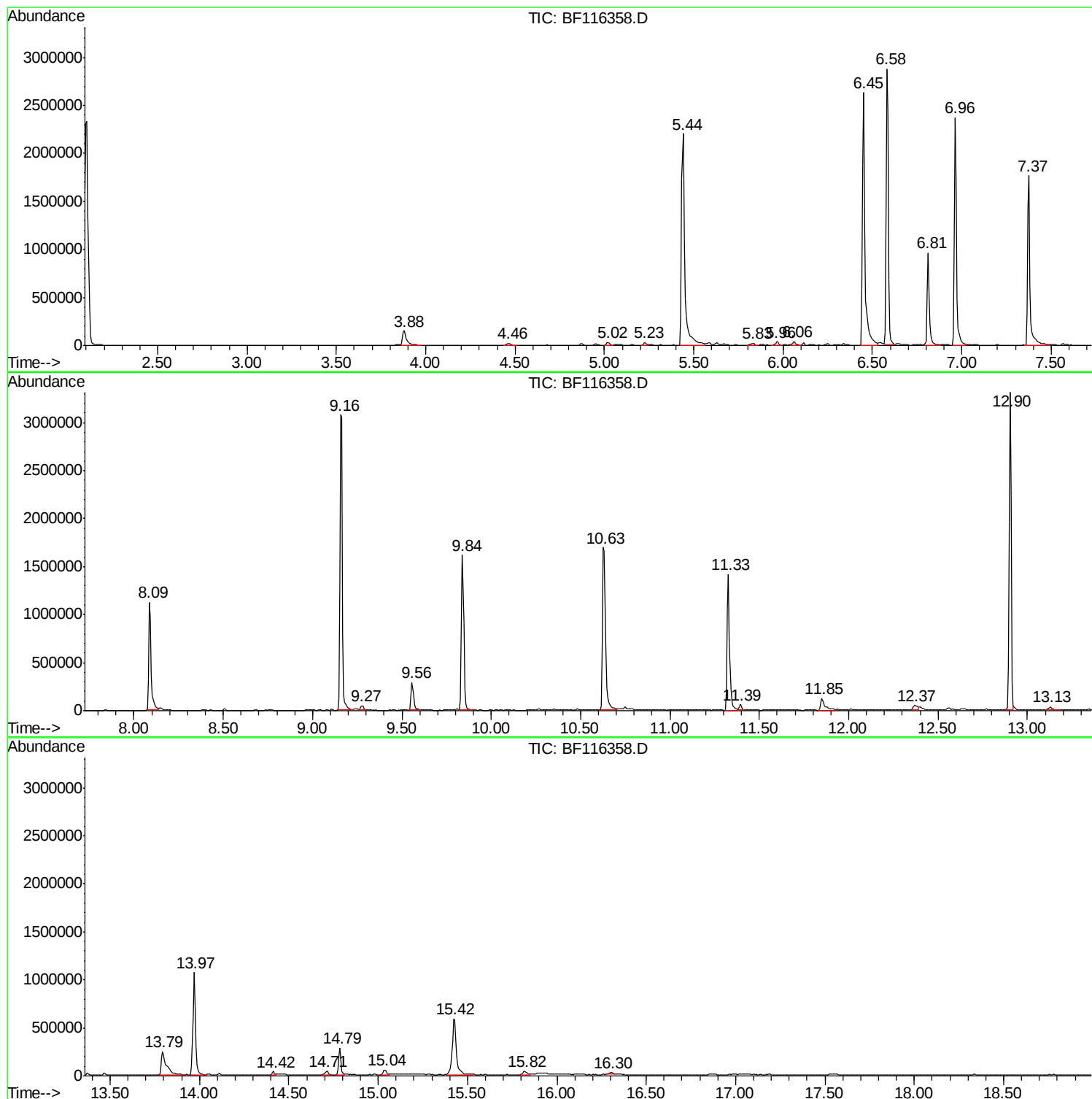
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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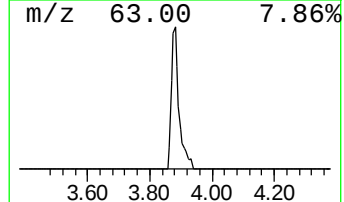
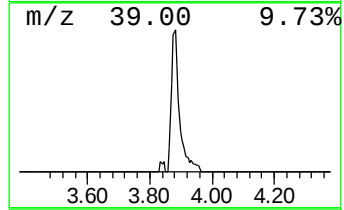
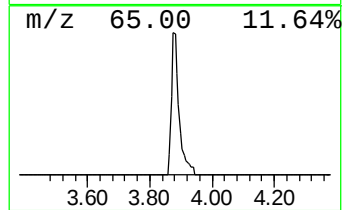
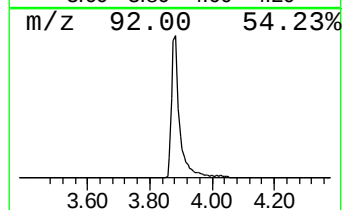
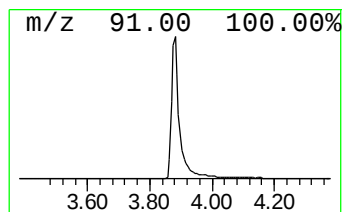
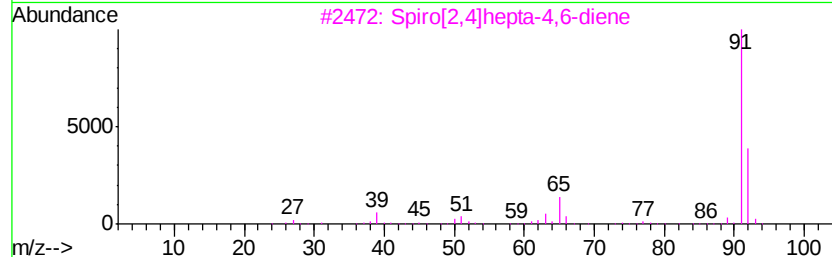
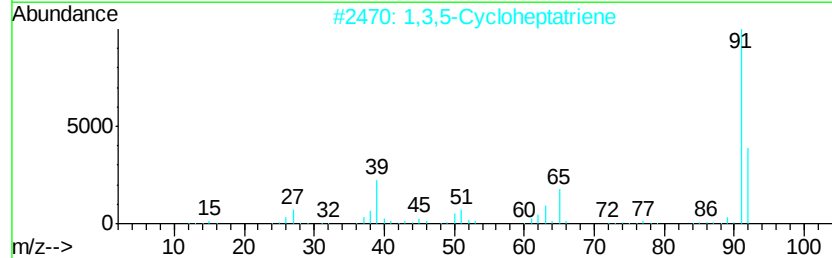
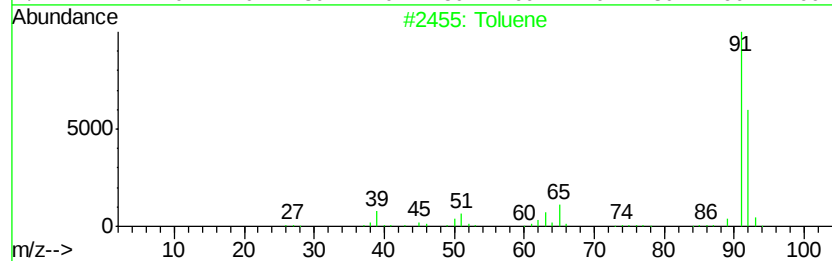
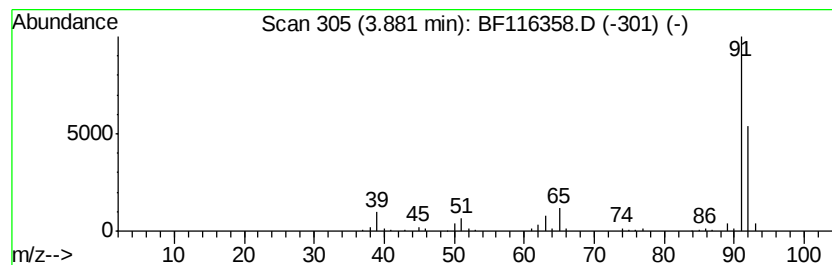
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 1,3,5-Cycloheptatriene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.88	5.66 ng	252231	1,4-Dichlorobenzene-d4	6.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Toluene	92	C7H8	000108-88-3	94
2			1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	86
3			Spiro[2.4]hepta-4,6-diene	92	C7H8	000765-46-8	76
4			Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	64
5			2,5-Norbornadiene	92	C7H8	000121-46-0	64



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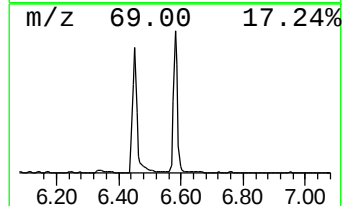
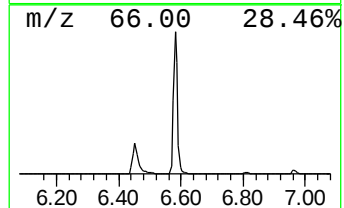
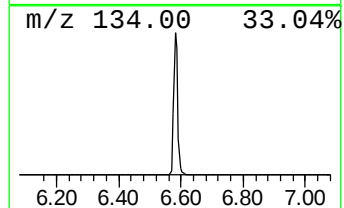
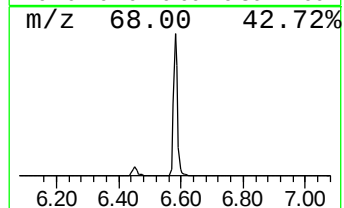
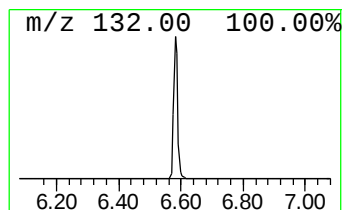
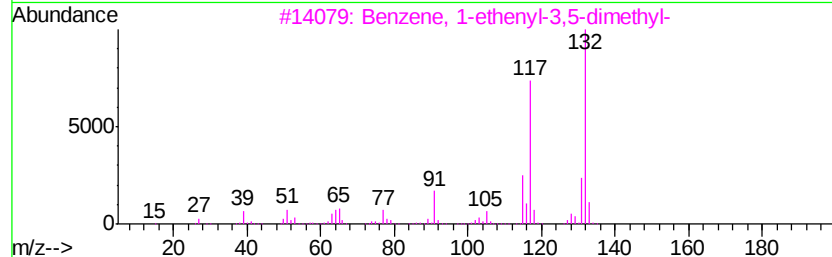
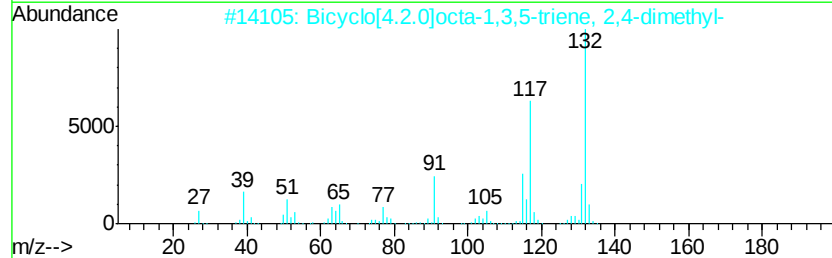
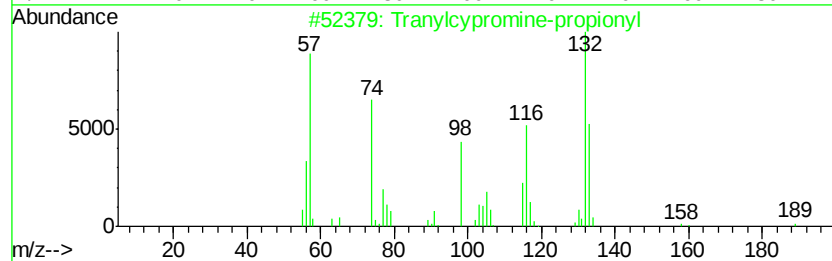
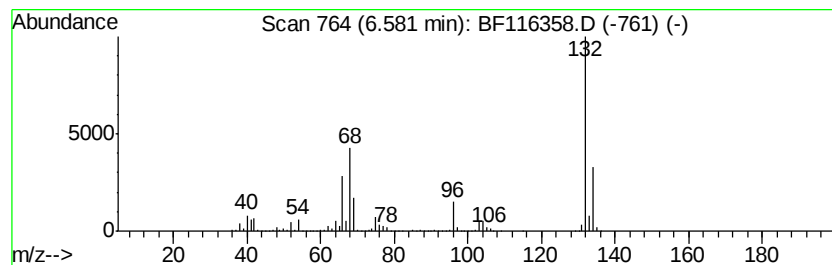
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	60.62 ng	2702340	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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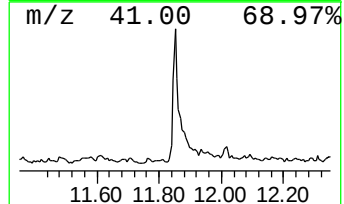
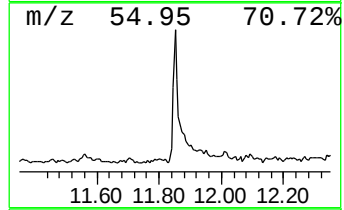
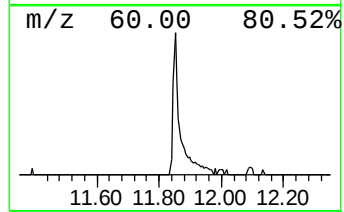
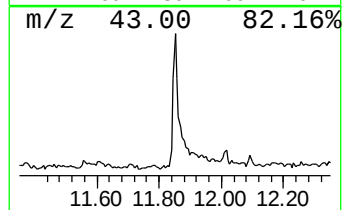
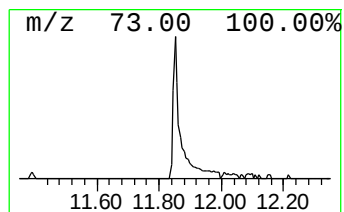
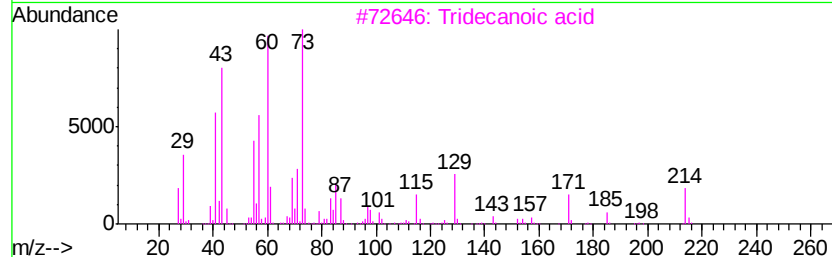
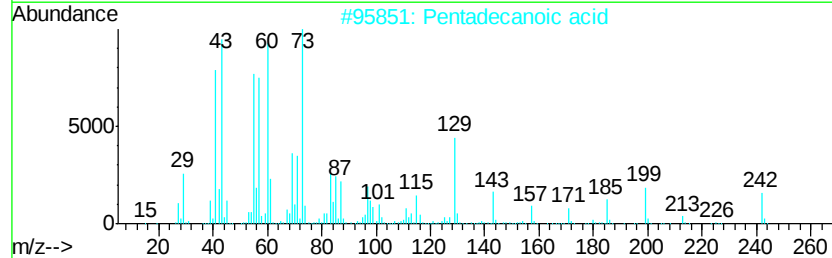
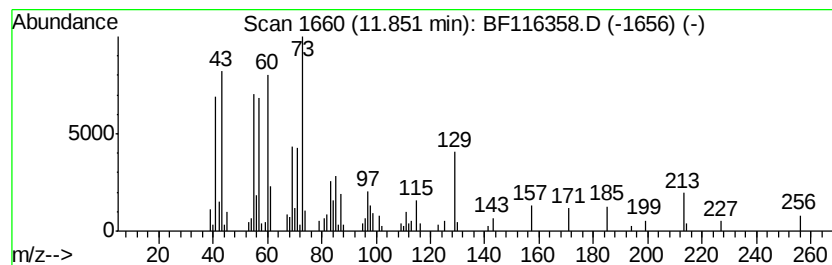
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	2.75 ng	183808	Phenanthrene-d10	11.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Tridecanoic acid	214	C13H26O2	000638-53-9	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	25



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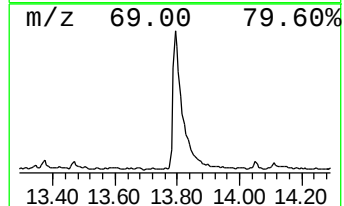
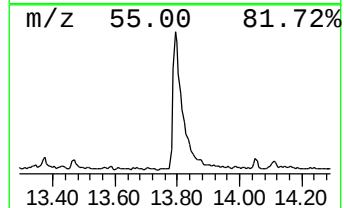
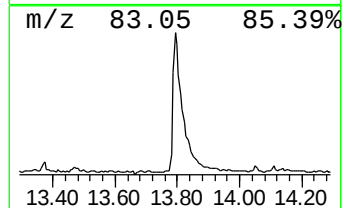
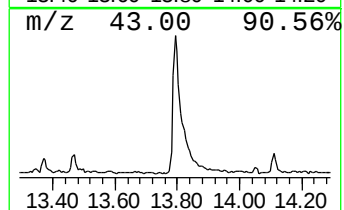
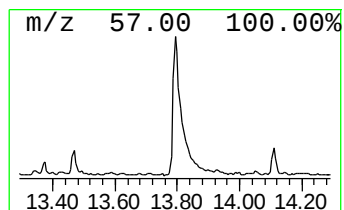
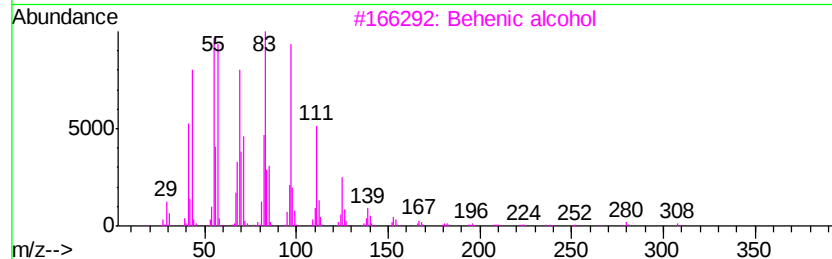
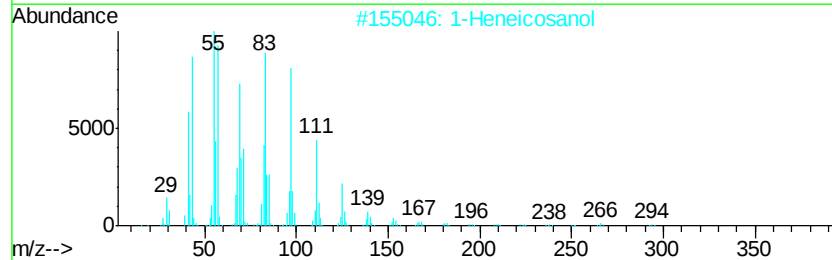
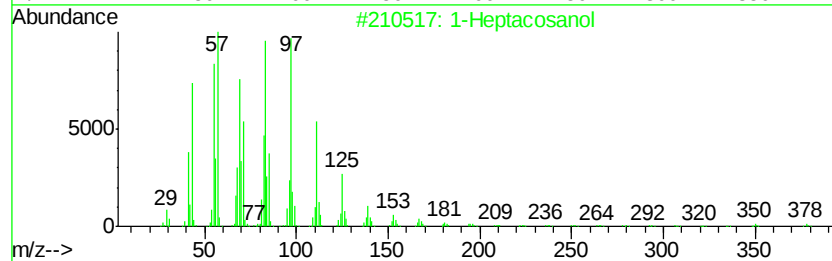
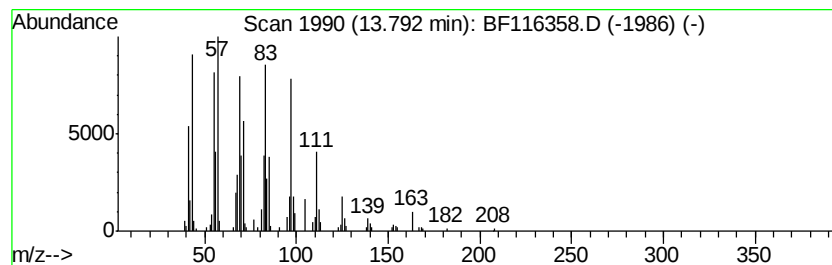
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Peak Number 5 1-Heptacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	10.07 ng	530620	Chrysene-d12	13.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heptacosanol	396	C27H56O	002004-39-9	94
2		1-Heneicosanol	312	C21H44O	015594-90-8	93
3		Behenic alcohol	326	C22H46O	000661-19-8	93
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	91



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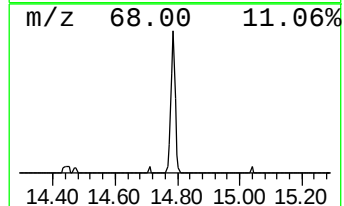
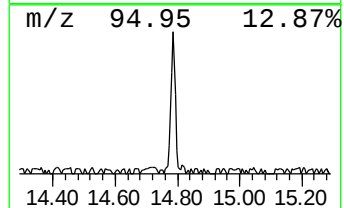
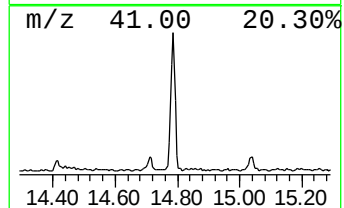
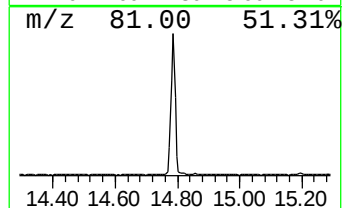
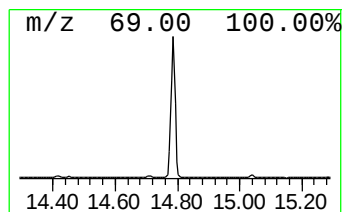
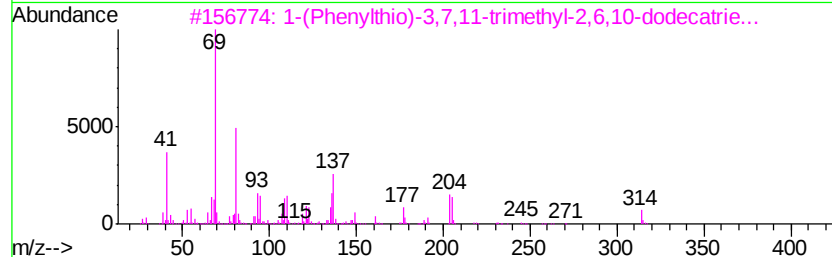
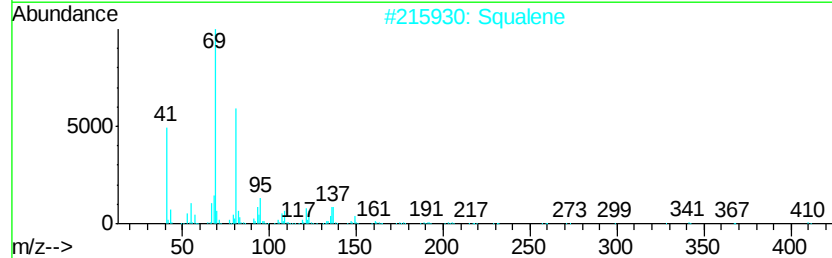
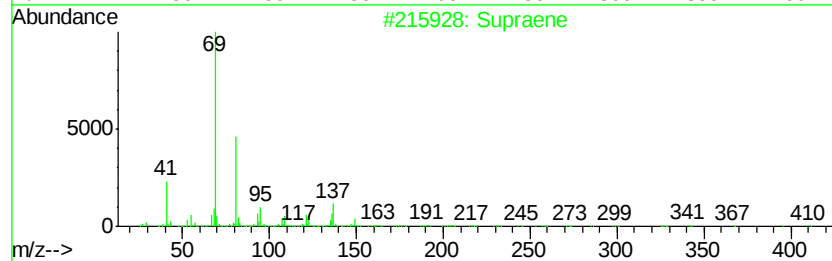
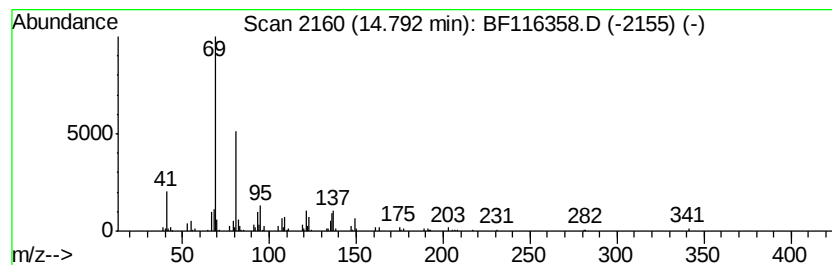
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Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	5.62 ng	262481	Perylene-d12	15.42

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		1-(Phenylthio)-3,7,11-trimethyl-...	314	C21H30S	028413-57-2	78
4		4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	52
5		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52



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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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
1,3,5-Cycloheptat...	3.88	5.7	ng	252231	1	6.81	891608	20.0
unknown6.58	6.58	60.6	ng	2702340	1	6.81	891608	20.0
n-Hexadecanoic acid	11.85	2.8	ng	183808	4	11.33	1338900	20.0
1-Heptacosanol	13.79	10.1	ng	530620	5	13.97	1054130	20.0
Squalene	14.79	5.6	ng	262481	6	15.42	933653	20.0