

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF073018\
 Data File : BF107807.D
 Acq On : 30 Jul 2018 18:33
 Operator : JU/SJ
 Sample : J4218-03
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-15-S

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-BF073018.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	496	rBV	425890	579258	12.68%	1.477%
2	5.595	551	554	576	rBV	1775481	2778819	60.85%	7.084%
3	6.595	721	724	744	rBV	1797893	3479654	76.20%	8.871%
4	6.731	744	747	783	rVV	2594715	4185897	91.66%	10.672%
5	6.960	783	786	808	rVV	574938	1183721	25.92%	3.018%
6	7.113	808	812	846	rVB	2278426	2824416	61.85%	7.201%
7	7.525	879	882	906	rBV	1155232	2221984	48.66%	5.665%
8	8.242	1000	1004	1033	rBV	917371	1441689	31.57%	3.676%
9	9.313	1182	1186	1219	rBV	3243517	4059378	88.89%	10.349%
10	9.707	1249	1253	1265	rBV	209417	250417	5.48%	0.638%
11	10.001	1298	1303	1321	rBV	1330882	1645556	36.03%	4.195%
12	10.795	1434	1438	1458	rBV	2099352	2983384	65.33%	7.606%
13	11.495	1553	1557	1580	rBV	1352536	1916847	41.98%	4.887%
14	12.001	1640	1643	1647	rBV	102614	113587	2.49%	0.290%
15	12.713	1760	1764	1774	rBV	73167	110015	2.41%	0.280%
16	12.948	1801	1804	1811	rVB	76772	93010	2.04%	0.237%
17	13.077	1822	1826	1847	rBV	3938157	4566635	100.00%	11.642%
18	13.283	1853	1861	1866	rBV3	47480	66672	1.46%	0.170%
19	13.624	1915	1919	1922	rBV	77742	72328	1.58%	0.184%
20	13.948	1971	1974	1990	rBV	349708	417423	9.14%	1.064%
21	14.148	2003	2008	2022	rBV	1286075	1877531	41.11%	4.787%
22	14.271	2026	2029	2033	rVB	110452	99132	2.17%	0.253%
23	14.571	2077	2080	2086	rBV	106665	134086	2.94%	0.342%
24	14.895	2130	2135	2139	rBV	106369	123545	2.71%	0.315%
25	14.977	2145	2149	2153	rBV	242917	260758	5.71%	0.665%
26	15.248	2187	2195	2207	rVB3	117502	224294	4.91%	0.572%
27	15.677	2263	2268	2284	rVB	680331	1306422	28.61%	3.331%
28	16.101	2336	2340	2346	rBV	54164	85523	1.87%	0.218%
29	16.636	2427	2431	2437	rBV2	34156	53102	1.16%	0.135%
30	17.265	2534	2538	2545	rVB9	31387	68970	1.51%	0.176%

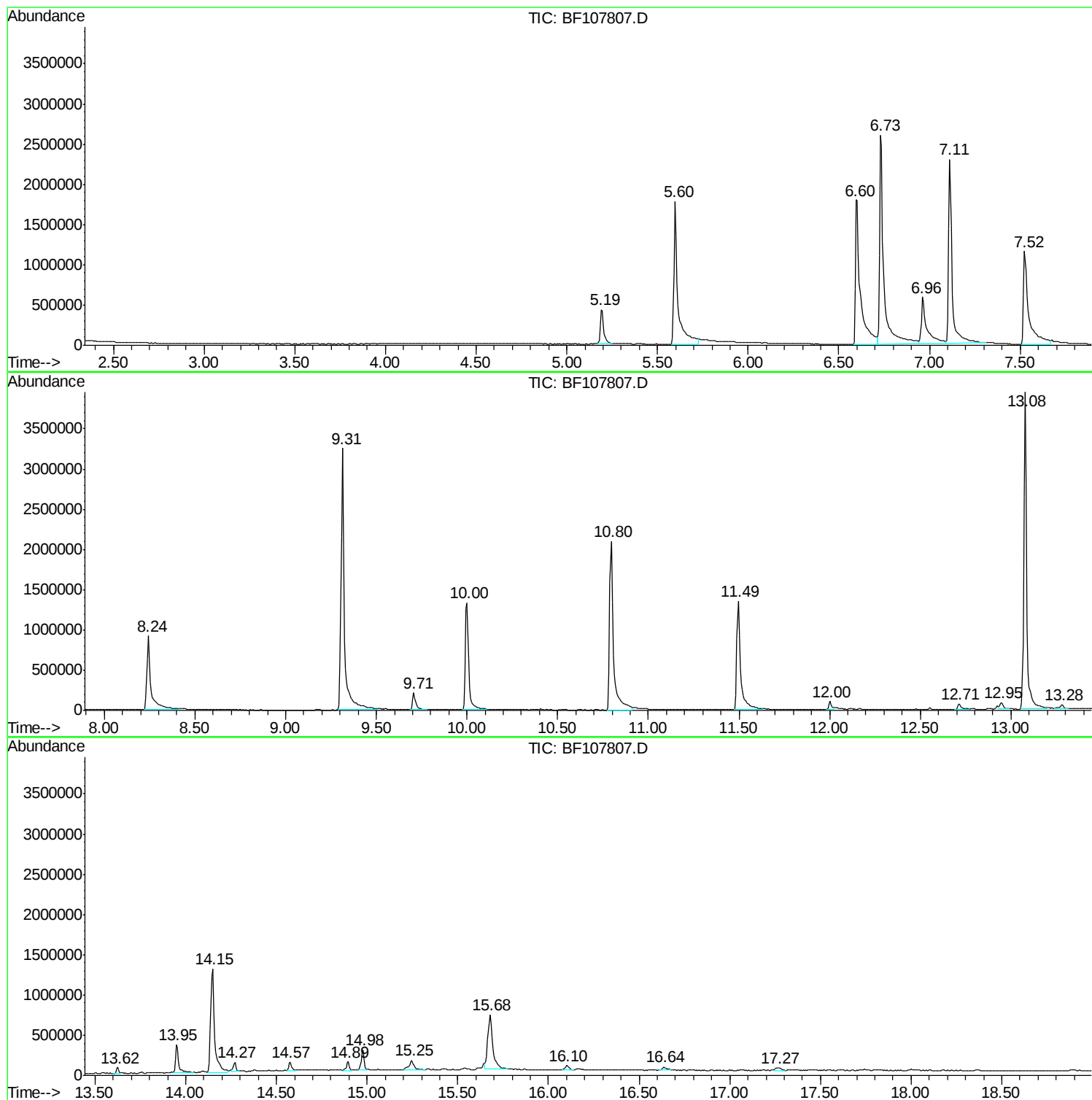
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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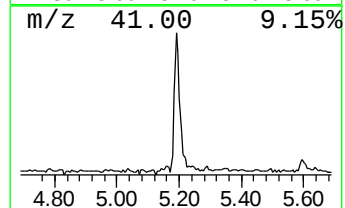
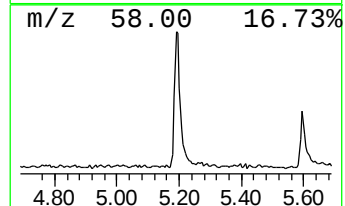
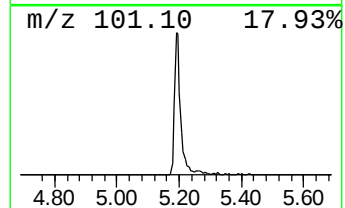
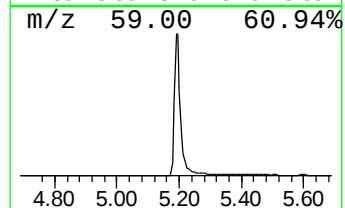
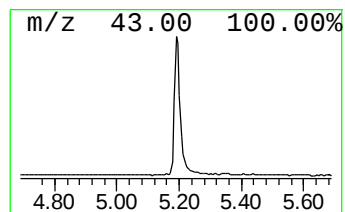
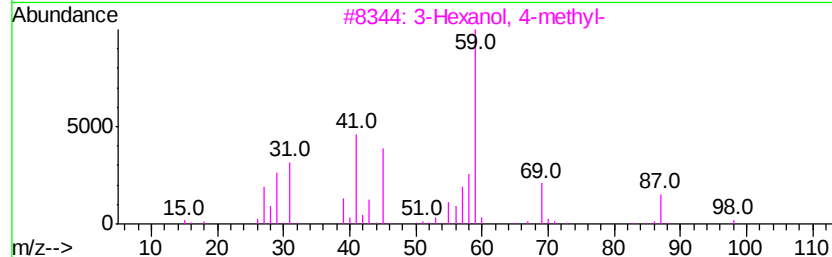
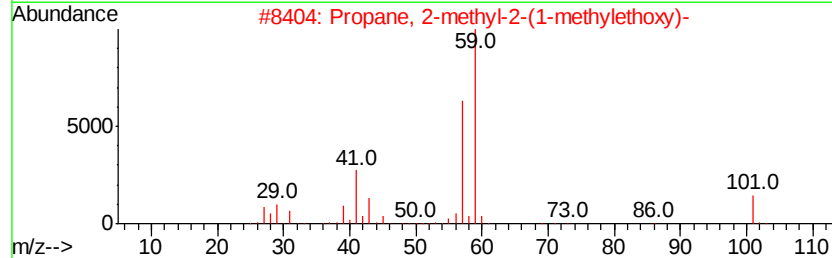
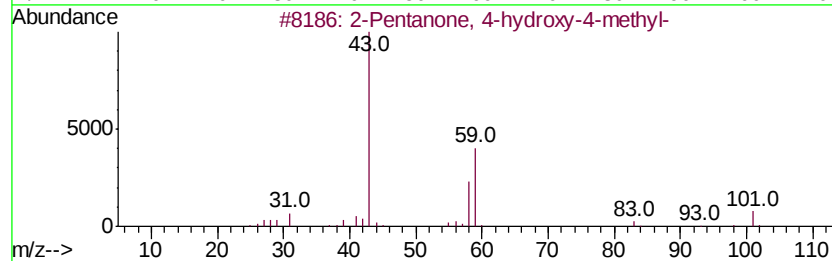
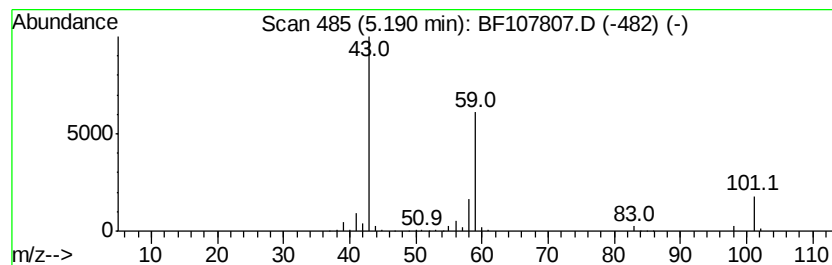
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	9.79 ng	579258	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	53
2		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	42
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	25



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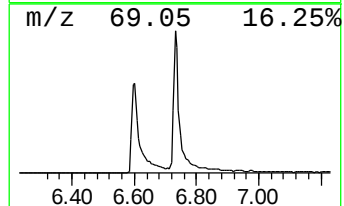
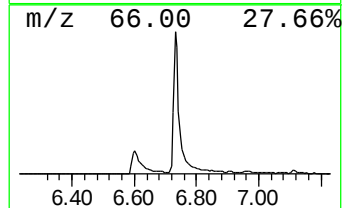
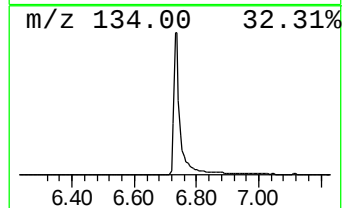
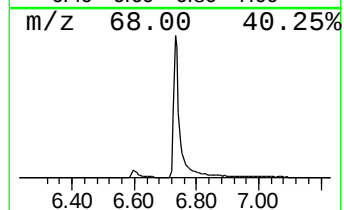
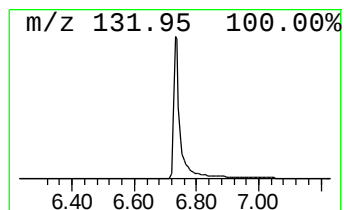
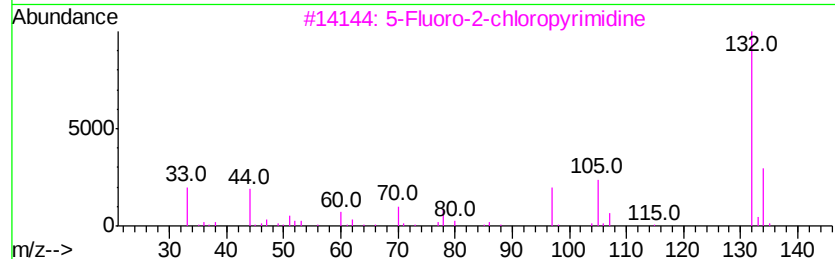
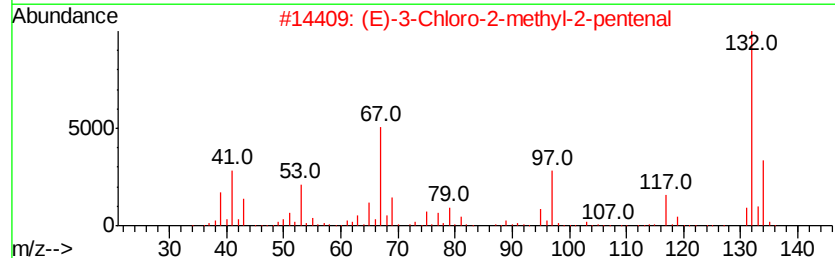
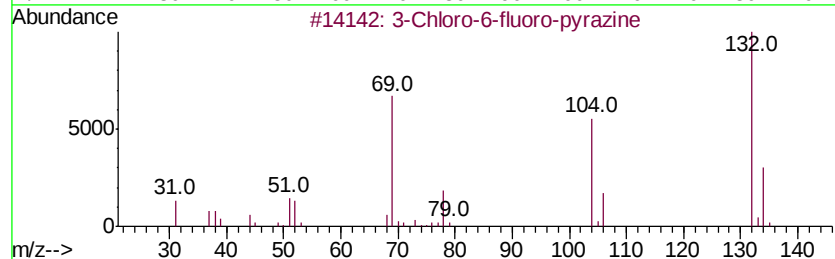
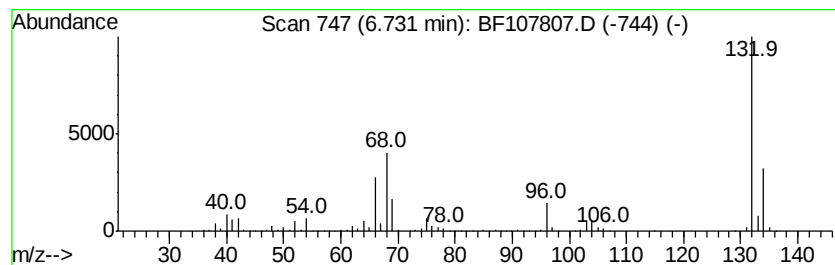
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Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	70.72 ng	4185900	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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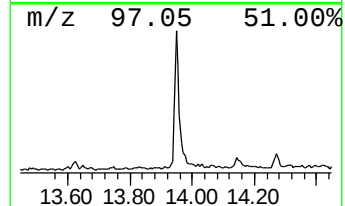
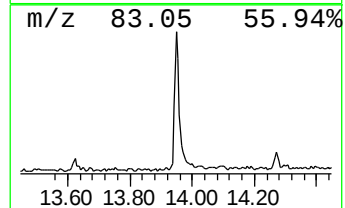
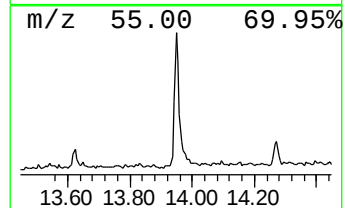
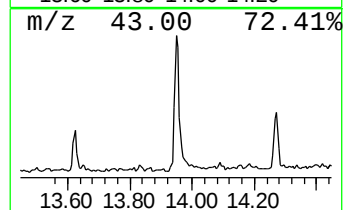
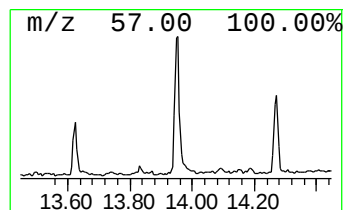
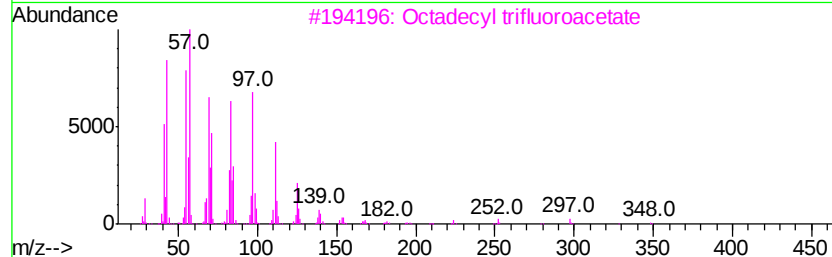
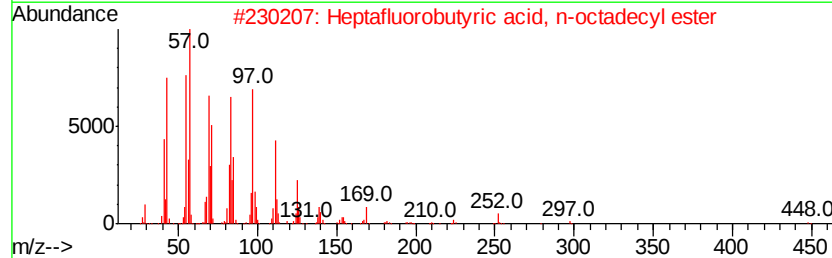
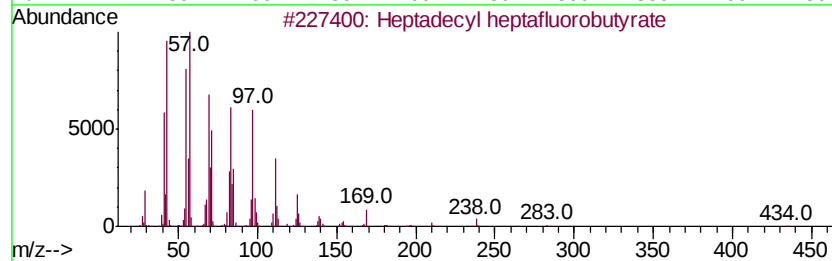
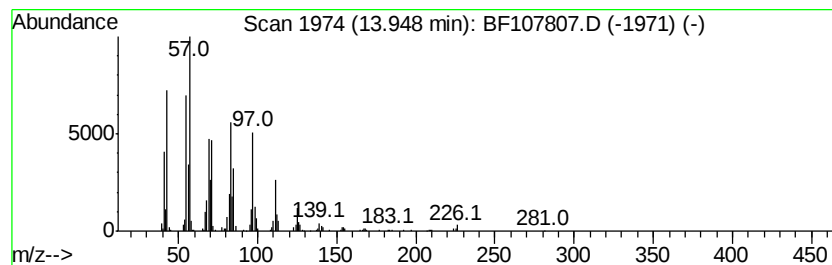
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	4.45 ng	417423	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2		Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	91
3		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
4		Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
5		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91



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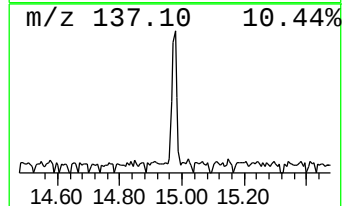
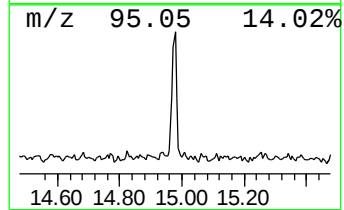
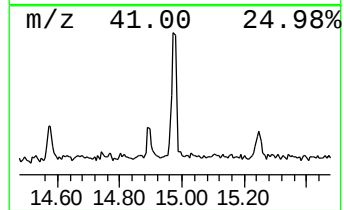
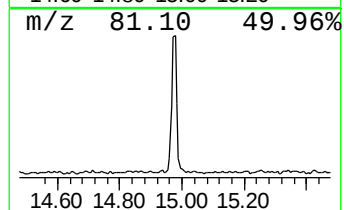
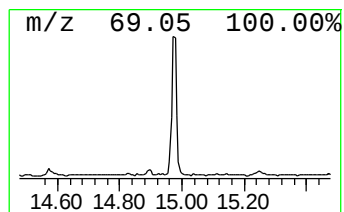
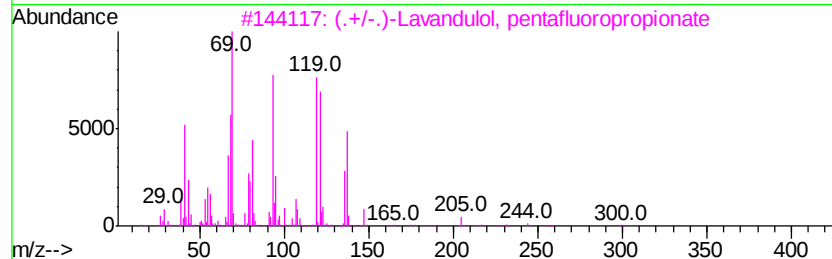
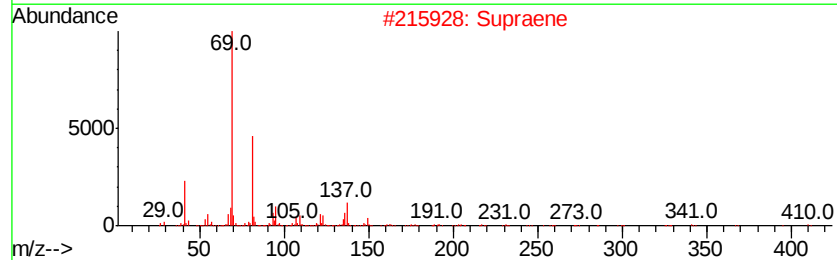
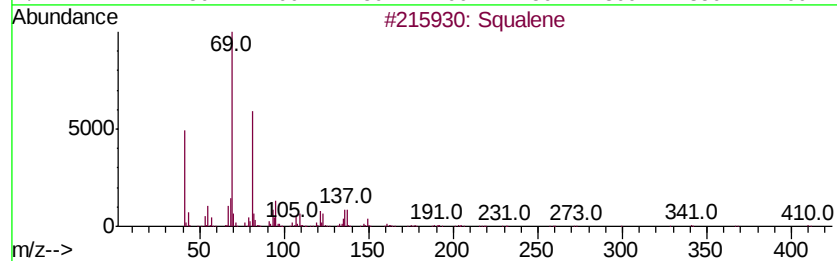
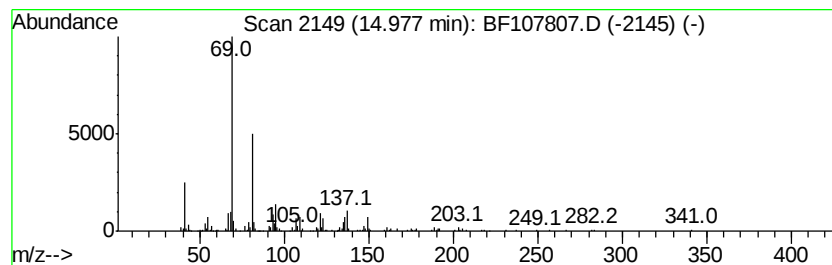
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Peak Number 5 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	3.99 ng	260758	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		(.+/-)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	72
4		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64



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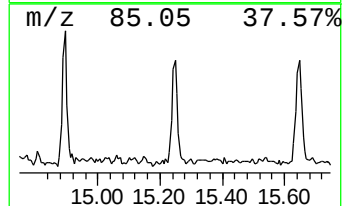
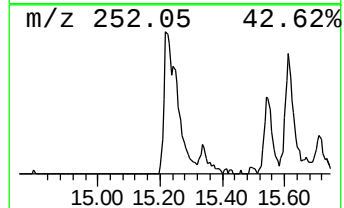
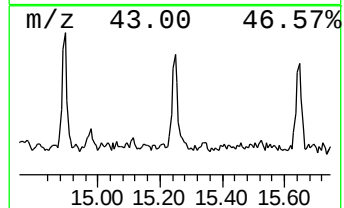
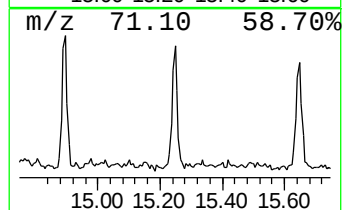
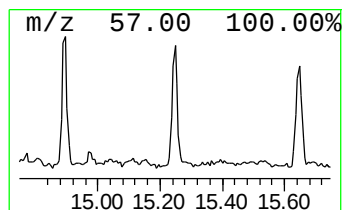
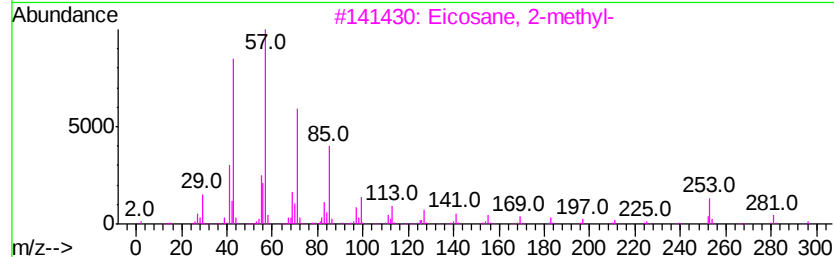
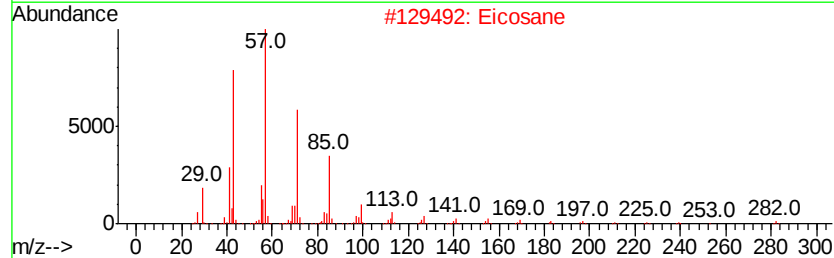
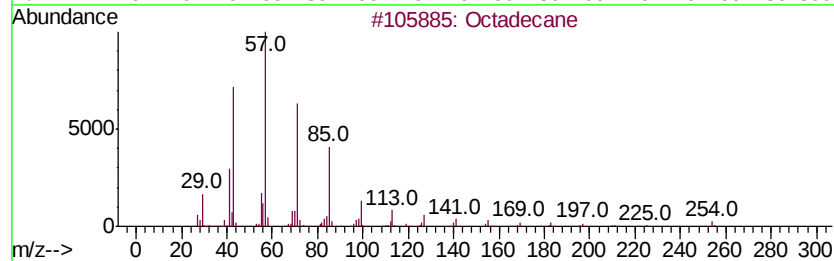
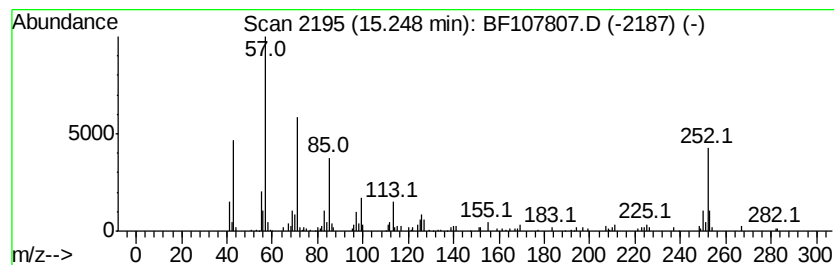
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TIC Library : C:\DATABASE\NIST11.L
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 Peak Number 6 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.25	3.43 ng	224294	Perylene-d12	15.68

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane		254	C18H38	000593-45-3	70
2	Eicosane		282	C20H42	000112-95-8	70
3	Eicosane, 2-methyl-		296	C21H44	001560-84-5	62
4	Pentacosane		352	C25H52	000629-99-2	53
5	Hexadecane		226	C16H34	000544-76-3	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.19	9.8	ng	579258	1	6.96	1183720	20.0
unknown6.73	6.73	70.7	ng	4185900	1	6.96	1183720	20.0
Heptadecyl heptaf...	13.95	4.5	ng	417423	5	14.15	1877530	20.0
Squalene	14.98	4.0	ng	260758	6	15.68	1306420	20.0
Octadecane	15.25	3.4	ng	224294	6	15.68	1306420	20.0