

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062618\
 Data File : BF106837.D
 Acq On : 26 Jun 2018 21:39
 Operator : JU/SJ
 Sample : J3570-02
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20180372-COMPOSITE-CS-1B

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	5.207	484	488	498	rBB	63864	78211	7.93%	0.880%
2	5.613	552	557	560	rBV	912167	928505	94.10%	10.447%
3	6.607	721	726	744	rBV	872320	986774	100.00%	11.102%
4	6.742	744	749	752	rBV	1009463	964395	97.73%	10.851%
5	6.960	783	786	789	rBV	313059	234477	23.76%	2.638%
6	7.119	809	813	816	rBV	913983	773913	78.43%	8.707%
7	7.525	877	882	885	rBV	620179	606217	61.43%	6.821%
8	8.242	1000	1004	1009	rBV	317619	267526	27.11%	3.010%
9	9.319	1182	1187	1195	rBV	936872	912275	92.45%	10.264%
10	9.707	1249	1253	1259	rVB	109780	94053	9.53%	1.058%
11	9.907	1284	1287	1292	rBV2	13352	13183	1.34%	0.148%
12	10.001	1300	1303	1311	rVB2	308517	272018	27.57%	3.061%
13	10.407	1370	1372	1375	rVB	18373	14411	1.46%	0.162%
14	10.795	1434	1438	1442	rBV	609442	556166	56.36%	6.258%
15	10.883	1450	1453	1455	rBV	13198	13027	1.32%	0.147%
16	10.907	1455	1457	1462	rVB	11762	12316	1.25%	0.139%
17	11.495	1553	1557	1560	rBV	345706	292360	29.63%	3.289%
18	11.519	1560	1561	1565	rVB	40202	23526	2.38%	0.265%
19	11.995	1640	1642	1645	rBV2	13042	13895	1.41%	0.156%
20	12.024	1645	1647	1651	rVB	13765	12110	1.23%	0.136%
21	12.107	1658	1661	1663	rBV2	10157	10824	1.10%	0.122%
22	12.130	1663	1665	1668	rVB	11117	10093	1.02%	0.114%
23	12.442	1713	1718	1720	rBV6	6900	12697	1.29%	0.143%
24	12.548	1733	1736	1739	rBV2	14111	13943	1.41%	0.157%
25	12.713	1761	1764	1767	rBV	40941	31338	3.18%	0.353%
26	12.924	1797	1800	1801	rBV2	13625	12698	1.29%	0.143%
27	12.942	1801	1803	1809	rVB	38970	46815	4.74%	0.527%
28	13.077	1822	1826	1830	rBV	978689	956117	96.89%	10.757%
29	13.471	1890	1893	1894	rBV	15131	12911	1.31%	0.145%
30	13.501	1896	1898	1901	rBV2	20934	27095	2.75%	0.305%
31	13.624	1917	1919	1922	rVB	14540	12885	1.31%	0.145%
32	13.960	1973	1976	1980	rVB	72669	76613	7.76%	0.862%
33	14.154	2005	2009	2011	rBV	336390	340773	34.53%	3.834%
34	14.283	2029	2031	2034	rVB	26819	18448	1.87%	0.208%

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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.695	2267	2271	2281	rVB	157775	235346	23.85%	2.648%
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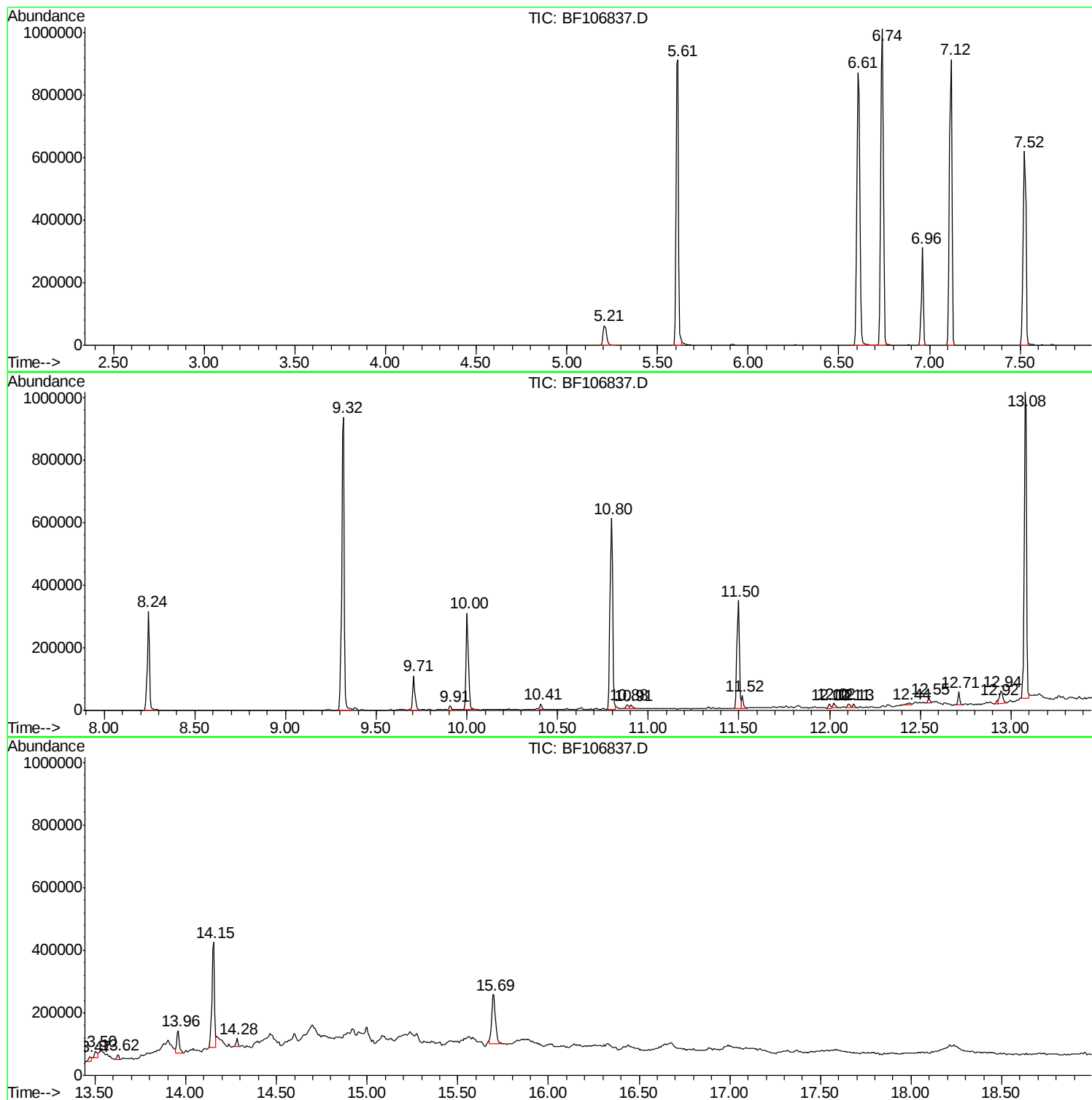
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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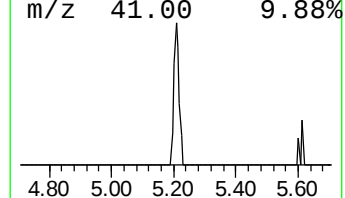
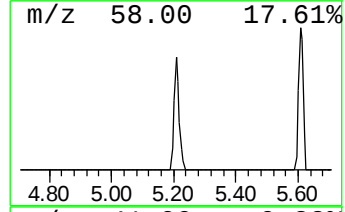
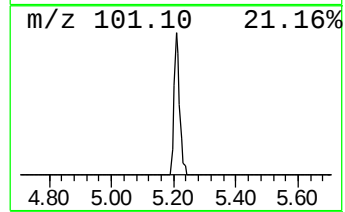
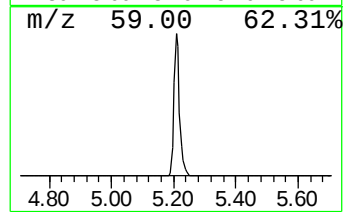
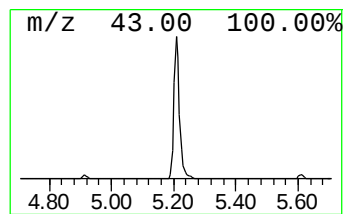
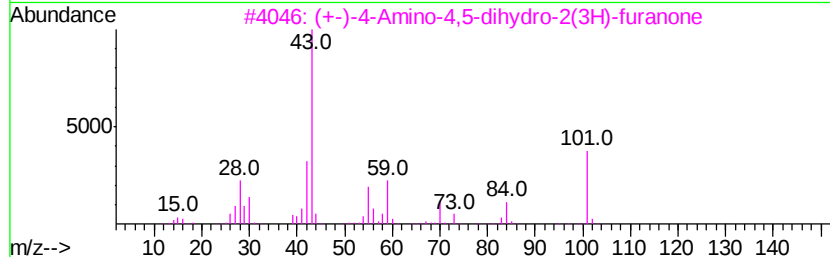
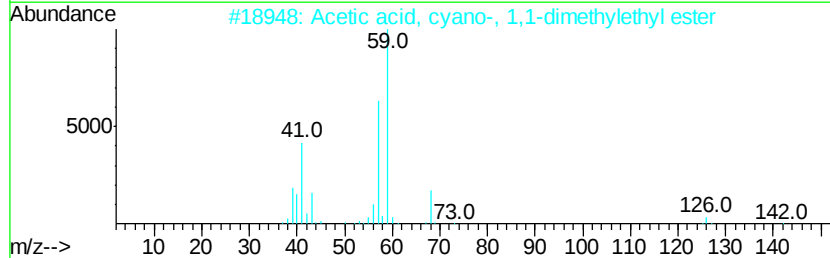
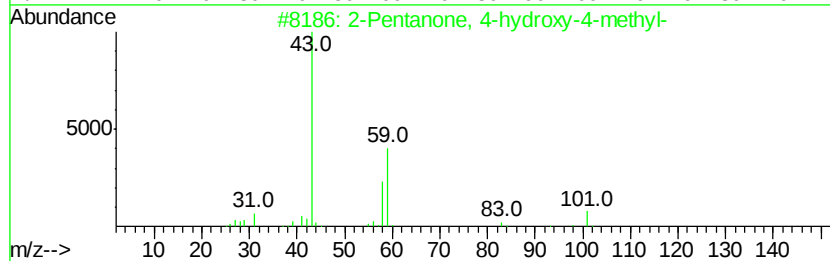
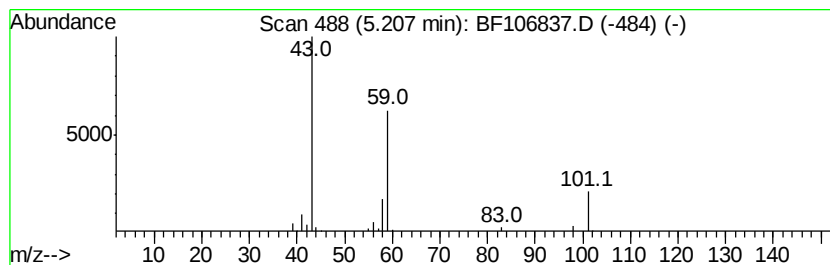
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	6.67 ng	78211	1,4-Dichlorobenzene-d4	6.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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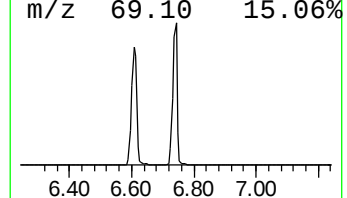
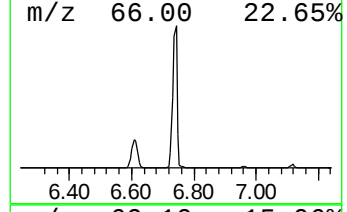
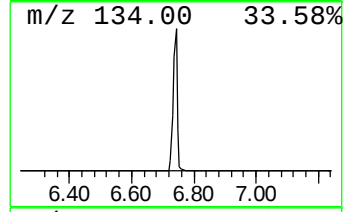
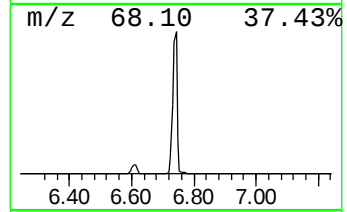
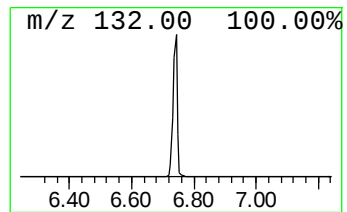
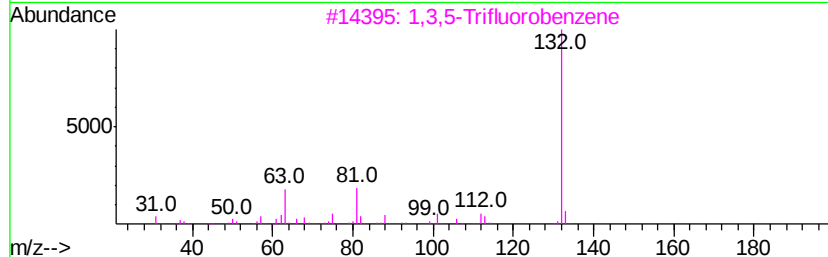
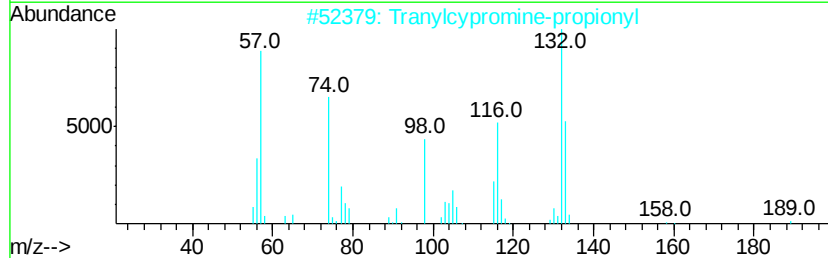
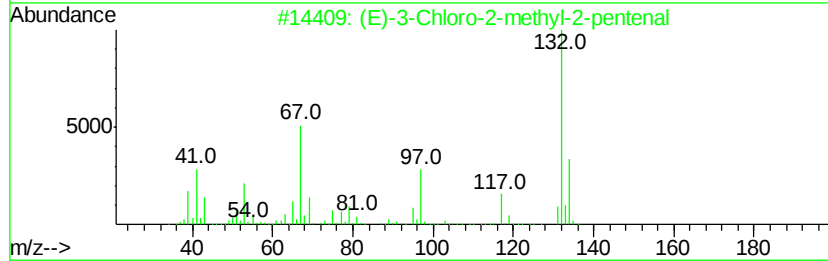
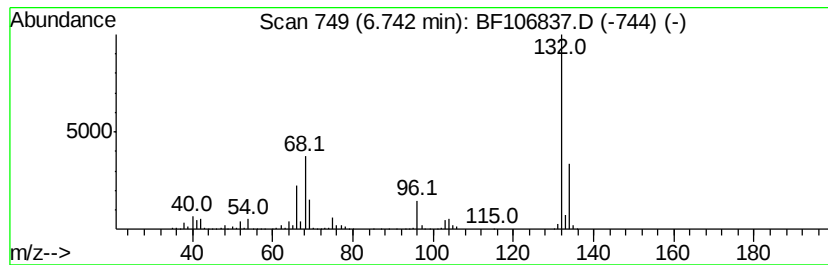
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	82.26 ng	964395	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		Xenon	132	Xe	007440-63-3	9
5		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9



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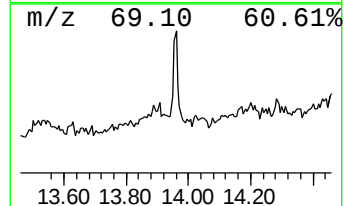
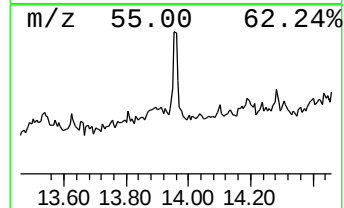
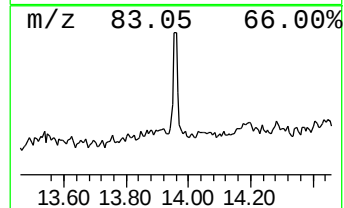
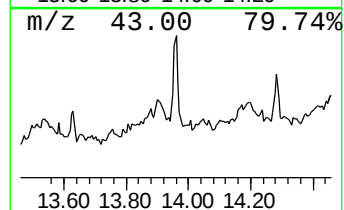
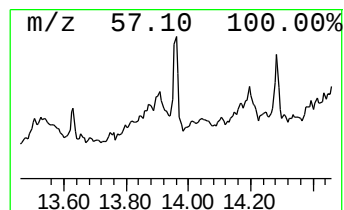
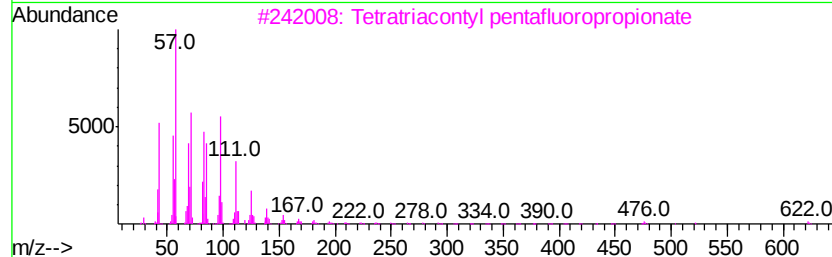
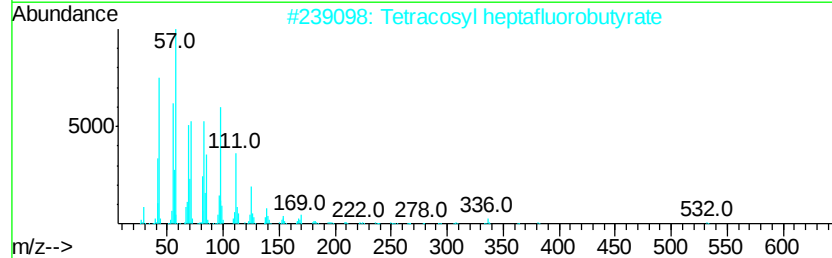
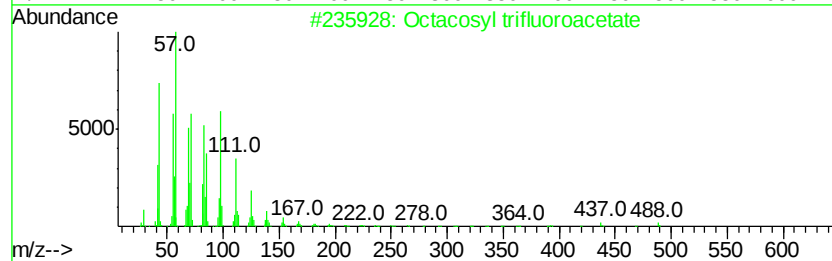
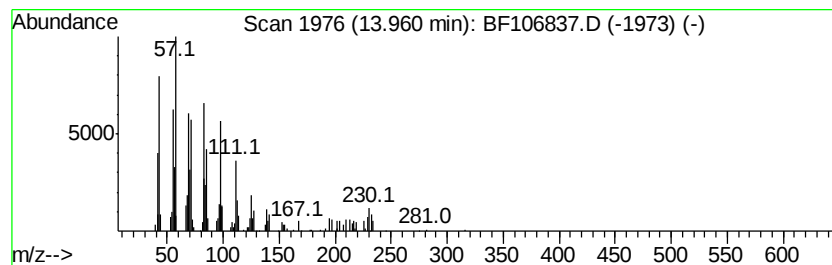
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Octacosyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	4.50 ng	76613	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
2		Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	87
3		Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	87
4		Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	87
5		Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.21	6.7	ng	78211	1	6.96	234477	20.0
unknown6.74	6.74	82.3	ng	964395	1	6.96	234477	20.0
Octacosyl trifluo...	13.96	4.5	ng	76613	5	14.15	340773	20.0