

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072418\
 Data File : BF107644.D
 Acq On : 25 Jul 2018 4:25
 Operator : JU/SJ
 Sample : J4120-05
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ST-4

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-BF072018.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	483	488	503	rBV	501208	713333	15.70%	1.762%
2	5.601	551	555	586	rBV	3136560	4508412	99.24%	11.138%
3	6.601	721	725	744	rBV	3165005	4507992	99.23%	11.137%
4	6.742	744	749	766	rVB	3814794	4543102	100.00%	11.223%
5	6.966	784	787	803	rBV	1167356	1451964	31.96%	3.587%
6	7.125	809	814	839	rBV	3022905	3541008	77.94%	8.748%
7	7.531	879	883	907	rBV	2253012	2883399	63.47%	7.123%
8	8.248	1001	1005	1035	rBV	1677264	1892902	41.67%	4.676%
9	9.325	1183	1188	1204	rBV	3849723	4221784	92.93%	10.430%
10	9.713	1251	1254	1260	rBV	196979	184266	4.06%	0.455%
11	10.007	1300	1304	1321	rBV2	1717305	1734982	38.19%	4.286%
12	10.801	1435	1439	1452	rBV	2119484	2322036	51.11%	5.736%
13	10.889	1452	1454	1461	rVB2	37646	54598	1.20%	0.135%
14	11.501	1554	1558	1567	rBV	1408238	1532435	33.73%	3.786%
15	12.007	1641	1644	1649	rBV3	44045	54630	1.20%	0.135%
16	13.083	1823	1827	1838	rBV	3129017	3084029	67.88%	7.619%
17	13.636	1918	1921	1924	rBV2	51177	48056	1.06%	0.119%
18	13.971	1974	1978	1986	rBV2	186541	261610	5.76%	0.646%
19	14.154	2004	2009	2018	rBV	1194230	1356298	29.85%	3.351%
20	14.283	2028	2031	2034	rBV	66333	60535	1.33%	0.150%
21	14.589	2080	2083	2086	rBV	68542	62431	1.37%	0.154%
22	14.907	2134	2137	2140	rBV	61331	60275	1.33%	0.149%
23	14.989	2148	2151	2155	rVB	121194	121521	2.67%	0.300%
24	15.265	2195	2198	2203	rVB	55916	69588	1.53%	0.172%
25	15.683	2263	2269	2280	rBV	686140	1106369	24.35%	2.733%
26	16.124	2342	2344	2351	rVB2	41456	53106	1.17%	0.131%
27	16.665	2433	2436	2442	rBV4	31304	48196	1.06%	0.119%

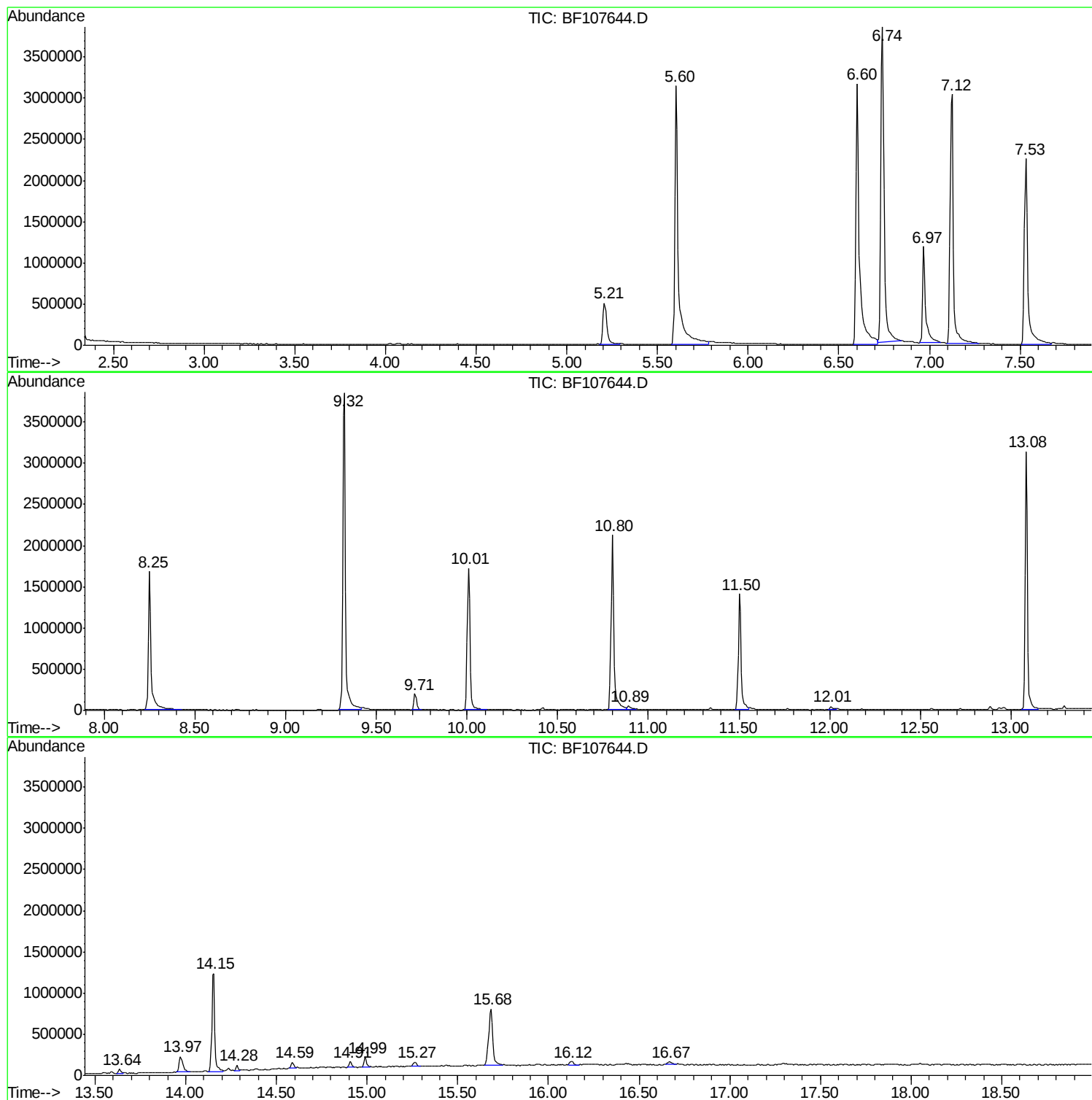
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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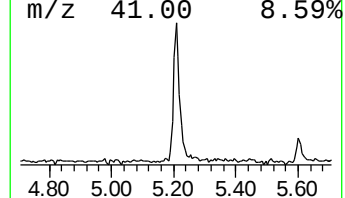
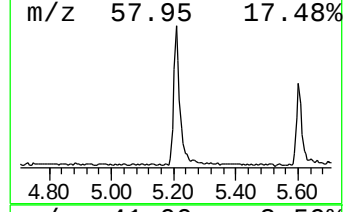
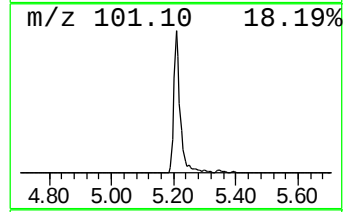
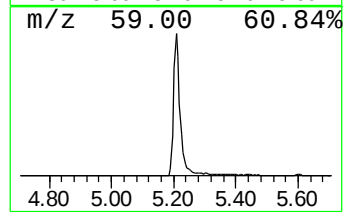
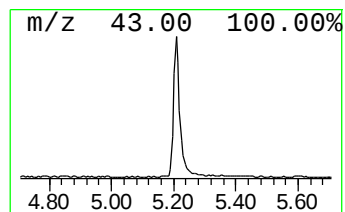
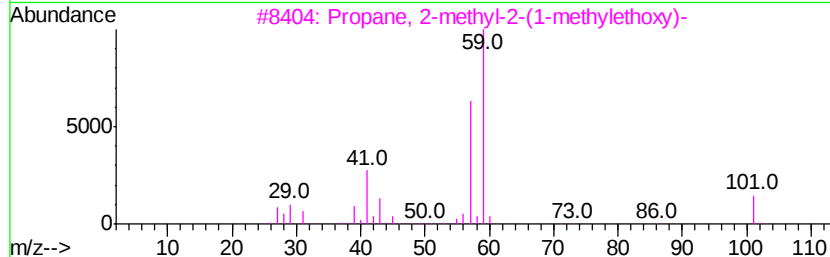
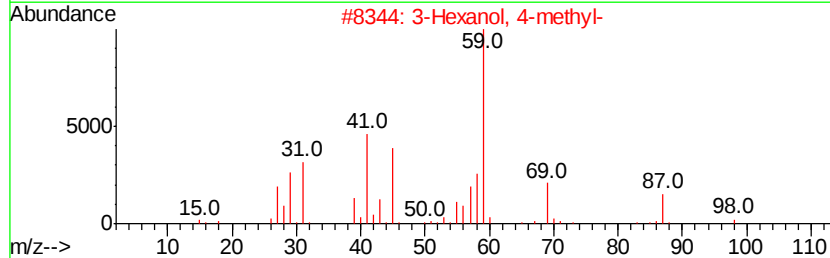
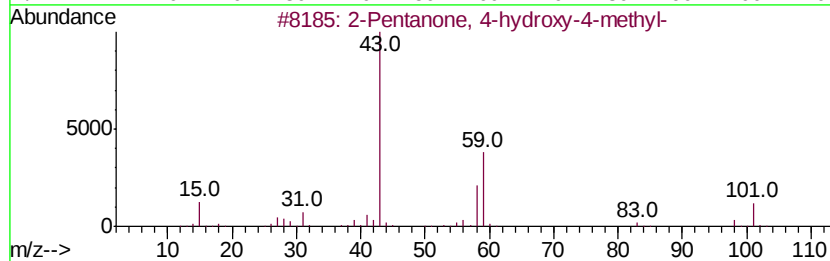
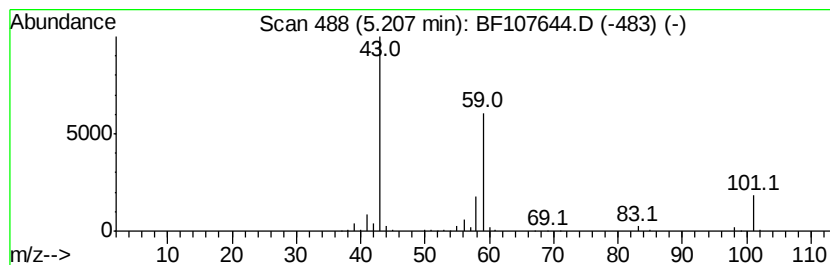
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	9.83 ng	713333	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5			Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	23



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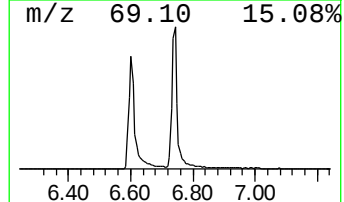
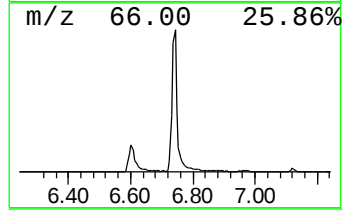
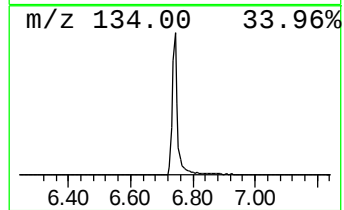
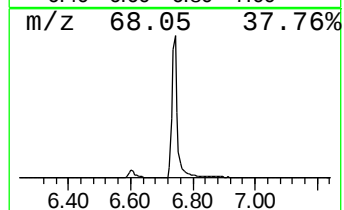
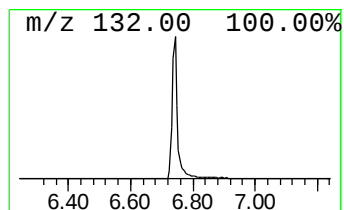
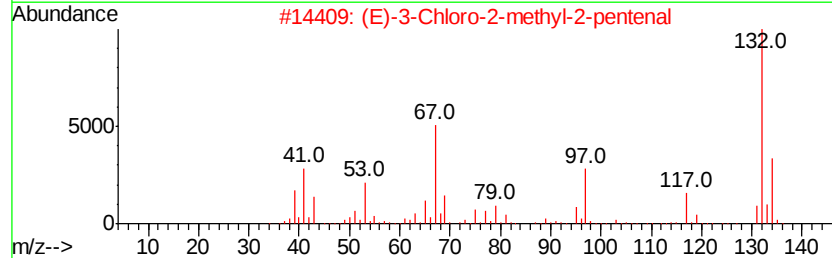
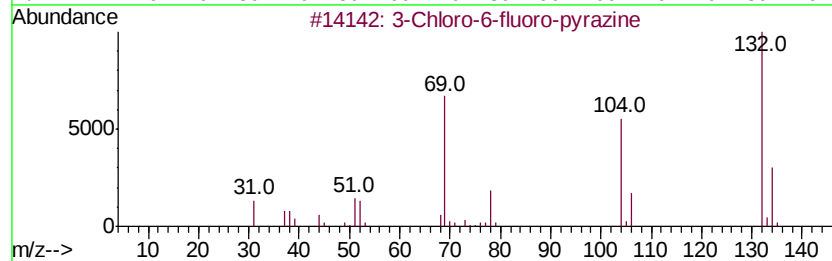
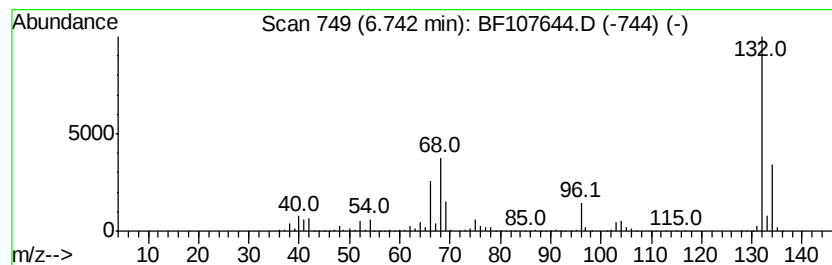
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Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	62.58 ng	4543100	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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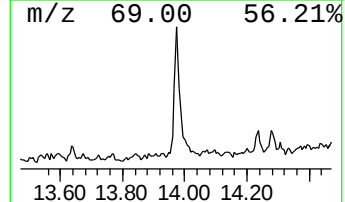
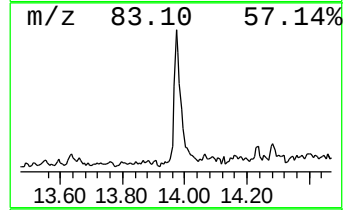
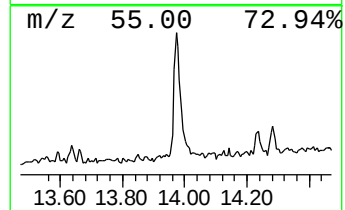
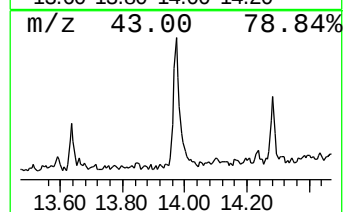
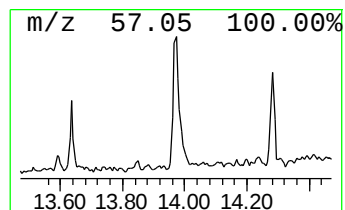
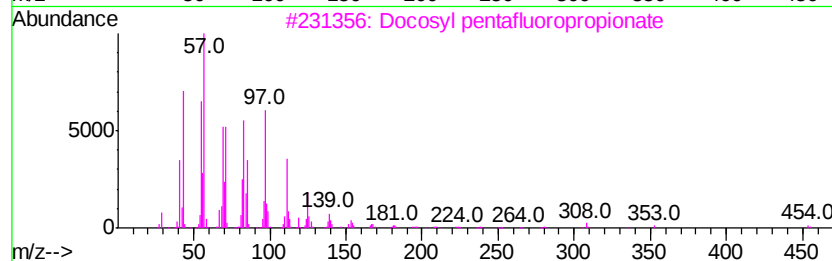
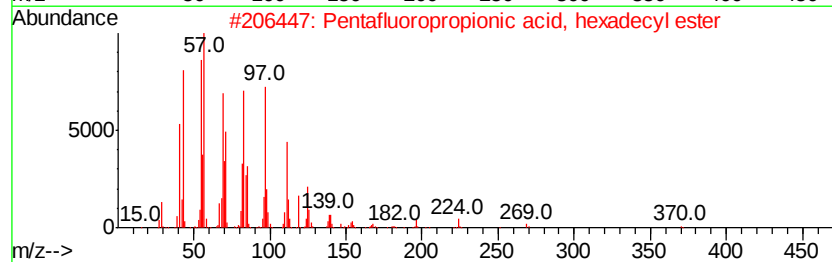
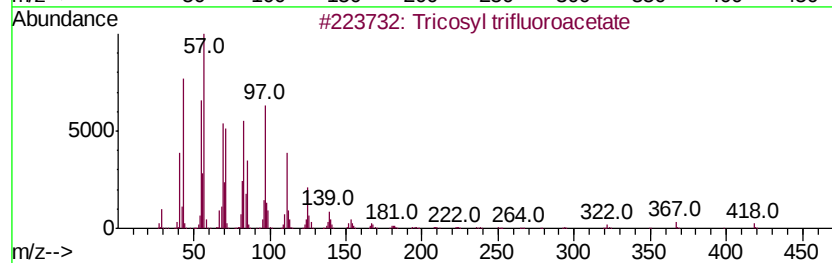
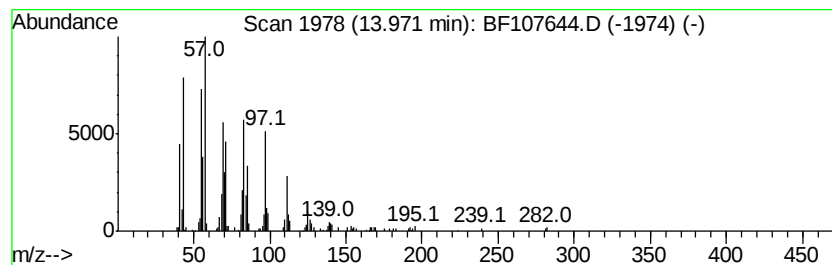
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Peak Number 4 Tricosyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	3.86 ng	261610	Chrysene-d12	14.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
2		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	90
3		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	90
4		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
5		Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	83



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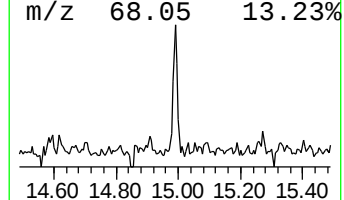
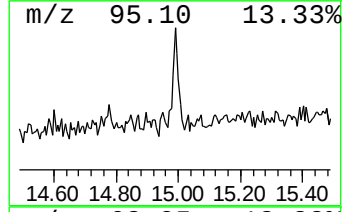
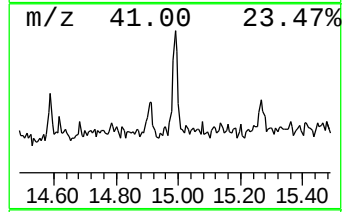
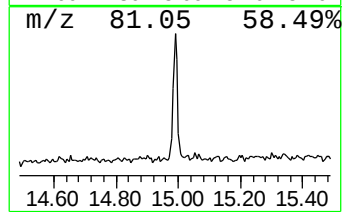
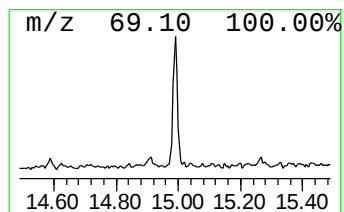
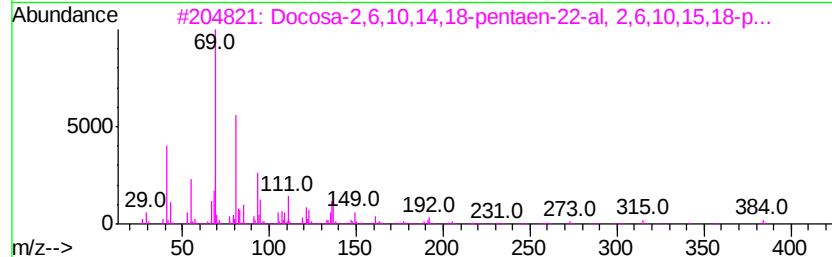
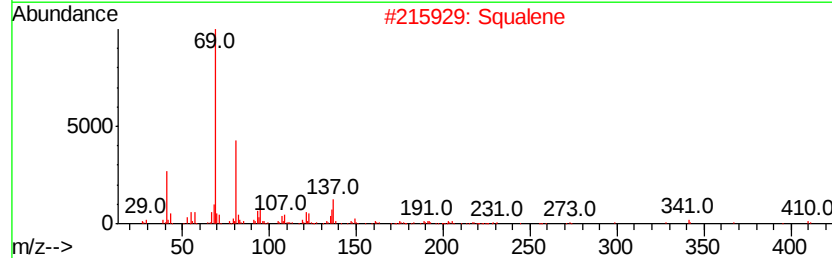
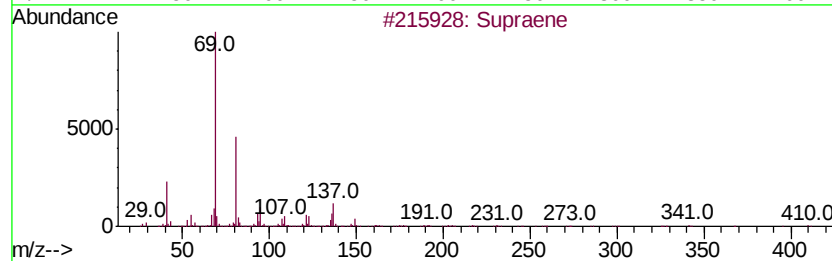
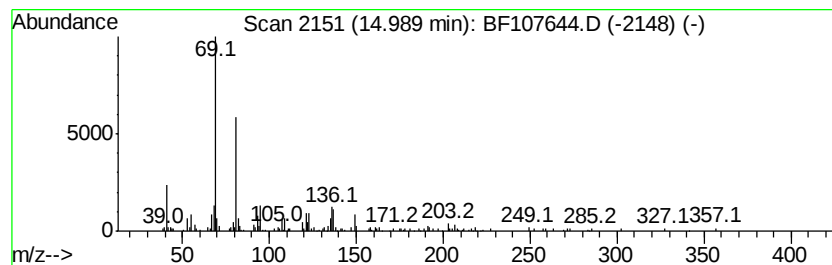
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 Peak Number 5 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	2.20 ng	121521	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	87
2		Squalene	410	C30H50	000111-02-4	87
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
4		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	78
5		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.21	9.8	ng	713333	1	6.97	1451960	20.0
unknown6.74	6.74	62.6	ng	4543100	1	6.97	1451960	20.0
Tricosyl trifluor...	13.97	3.9	ng	261610	5	14.15	1356300	20.0
Supraene	14.99	2.2	ng	121521	6	15.68	1106370	20.0