

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF073018\
 Data File : BF107812.D
 Acq On : 30 Jul 2018 20:46
 Operator : JU/SJ
 Sample : J4164-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-6(3-5)

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	5.201	483	487	504	rBV	597101	873807	15.06%	1.722%
2	5.601	551	555	584	rBV	3200485	4707155	81.12%	9.277%
3	6.607	722	726	744	rBV	2957706	4889264	84.26%	9.636%
4	6.737	744	748	783	rVV	3997994	5671891	97.75%	11.178%
5	6.960	783	786	808	rVV	702354	1237395	21.33%	2.439%
6	7.113	808	812	839	rVV	3292866	3925599	67.65%	7.737%
7	7.525	878	882	906	rBV	1981001	3306859	56.99%	6.517%
8	8.242	1000	1004	1034	rBV	1118025	1612710	27.79%	3.178%
9	9.313	1181	1186	1220	rBV	4507845	5802461	100.00%	11.436%
10	9.707	1248	1253	1263	rBV	256574	295064	5.09%	0.582%
11	10.001	1298	1303	1318	rBV	1478111	1706757	29.41%	3.364%
12	10.795	1434	1438	1463	rBV	2839862	3993911	68.83%	7.871%
13	11.495	1553	1557	1570	rBV	1409603	1903754	32.81%	3.752%
14	12.001	1640	1643	1647	rBV	133655	154146	2.66%	0.304%
15	12.713	1761	1764	1771	rBV	119008	169118	2.91%	0.333%
16	12.948	1801	1804	1810	rVB	113999	136065	2.34%	0.268%
17	13.077	1822	1826	1847	rBV	4232997	5458962	94.08%	10.759%
18	13.283	1858	1861	1864	rVB2	70104	65612	1.13%	0.129%
19	13.624	1916	1919	1922	rBV	109926	109188	1.88%	0.215%
20	13.954	1971	1975	1981	rBV	363218	410104	7.07%	0.808%
21	14.148	2003	2008	2021	rBV2	1147841	1809950	31.19%	3.567%
22	14.271	2026	2029	2032	rVB	137994	126286	2.18%	0.249%
23	14.577	2078	2081	2086	rBV	155833	152276	2.62%	0.300%
24	14.895	2133	2135	2138	rVB	172795	146396	2.52%	0.289%
25	14.977	2146	2149	2152	rVB	283665	260401	4.49%	0.513%
26	15.248	2193	2195	2201	rVB	166123	193595	3.34%	0.382%
27	15.613	2254	2257	2260	rBV2	90575	148463	2.56%	0.293%
28	15.677	2265	2268	2281	rVB	755019	1331745	22.95%	2.625%
29	16.107	2338	2341	2346	rVB	95749	140387	2.42%	0.277%

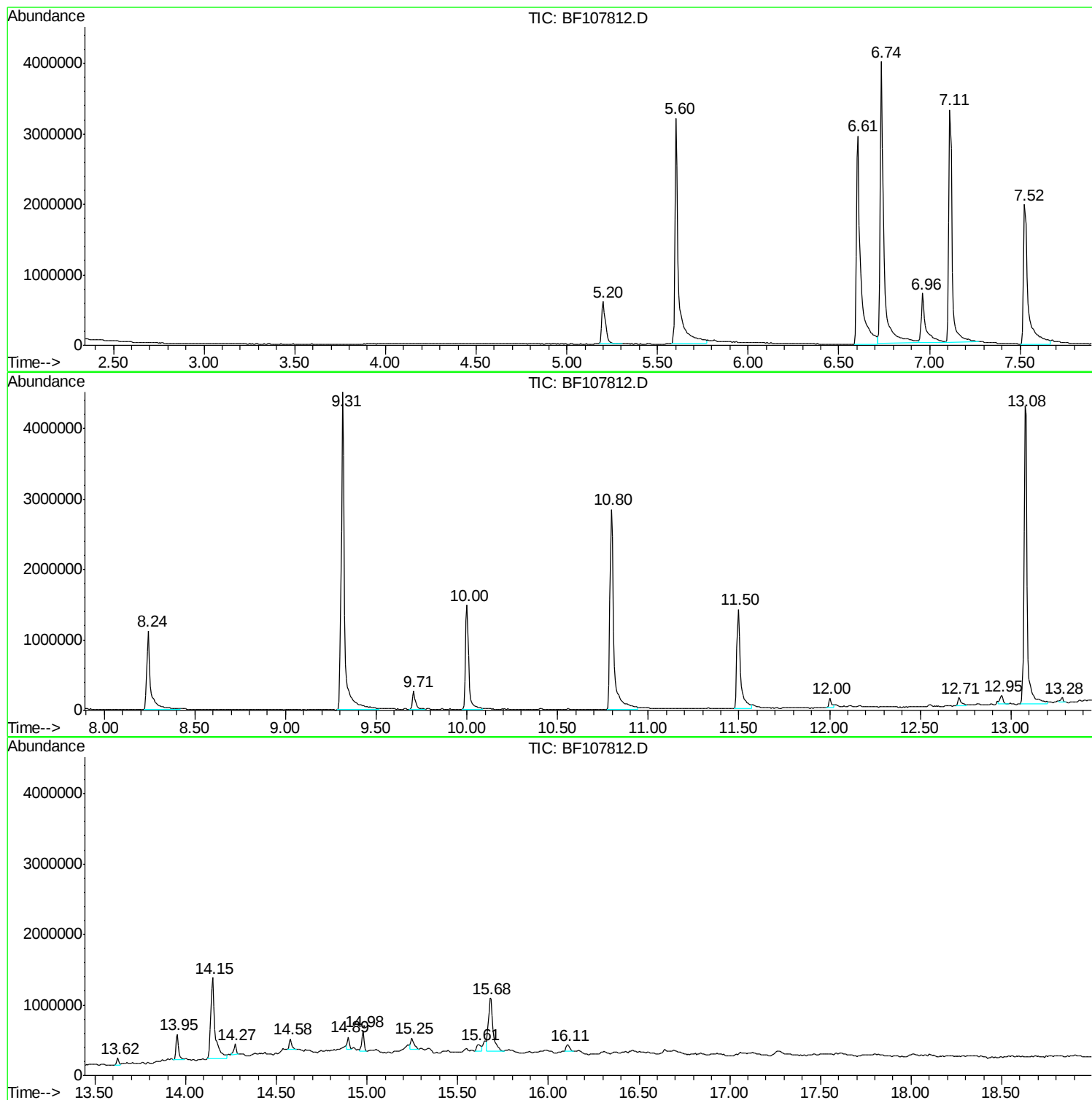
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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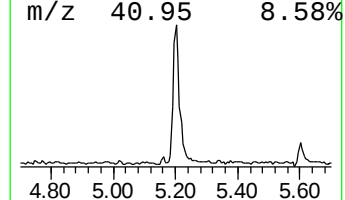
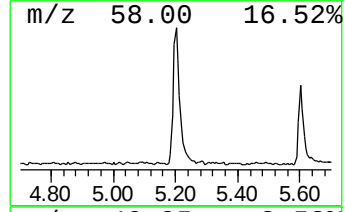
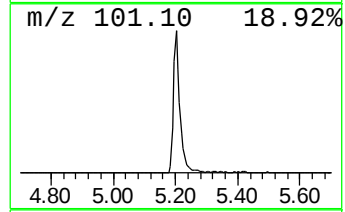
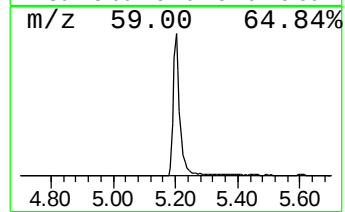
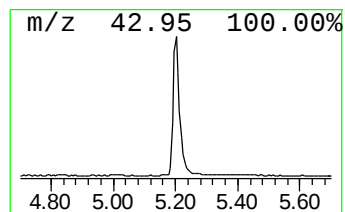
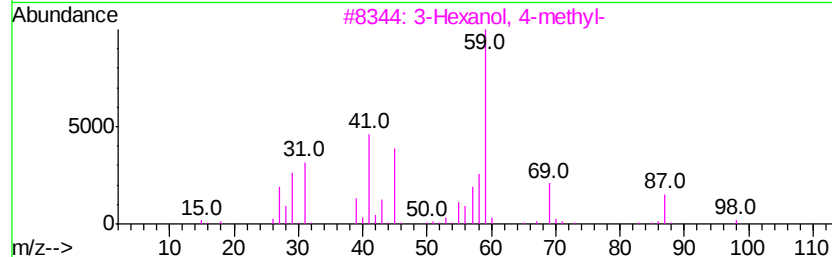
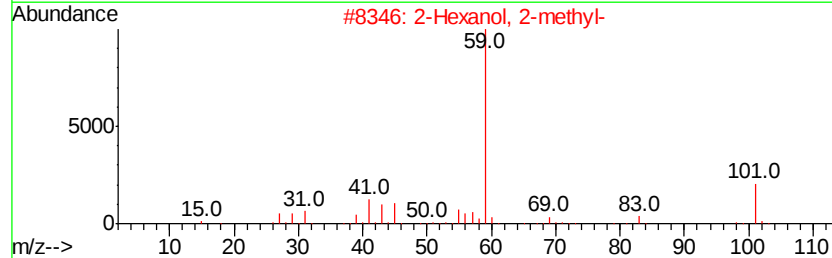
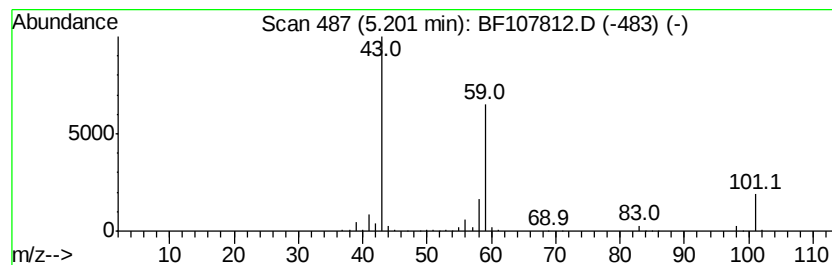
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	14.12 ng	873807	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	50
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Propane, 2-methyl-2-(1-methylethyl)-	116	C7H16O	017348-59-3	33
5			Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	25



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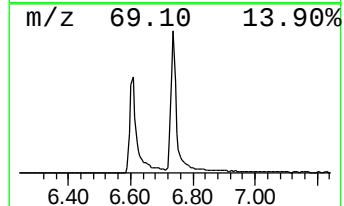
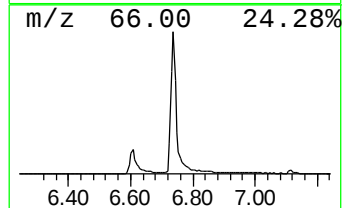
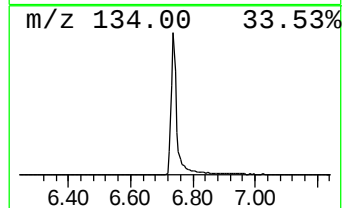
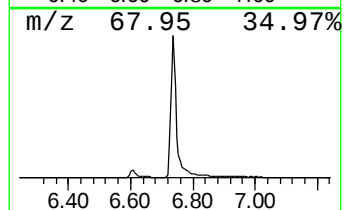
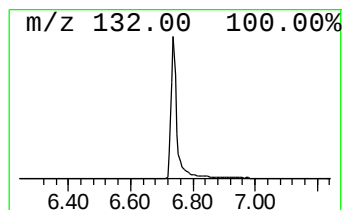
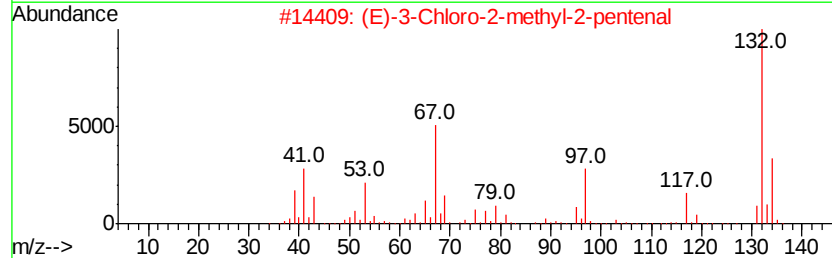
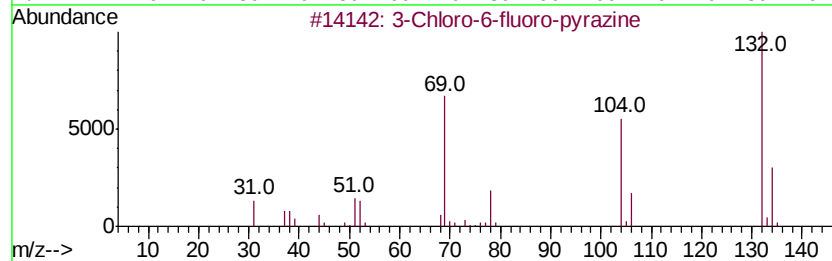
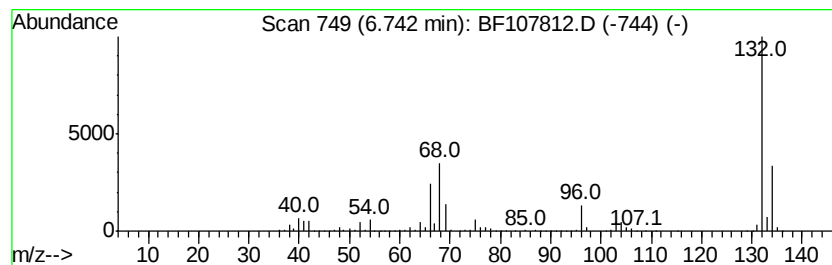
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TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	91.67 ng	5671890	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	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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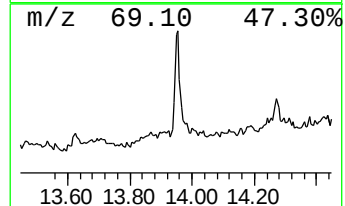
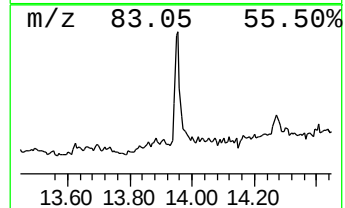
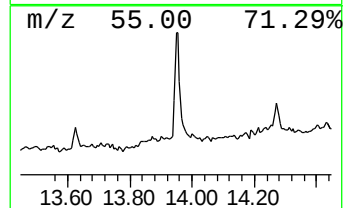
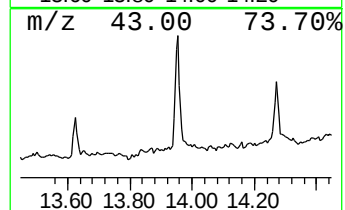
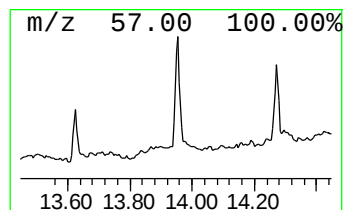
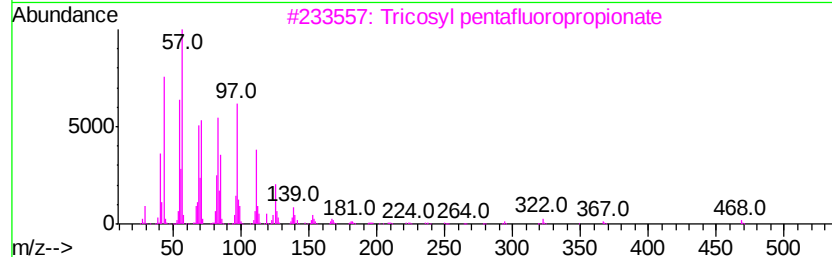
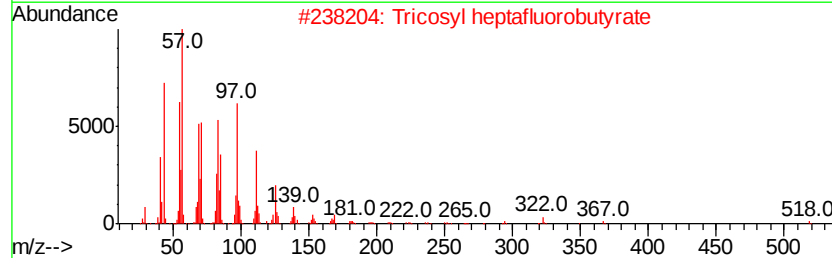
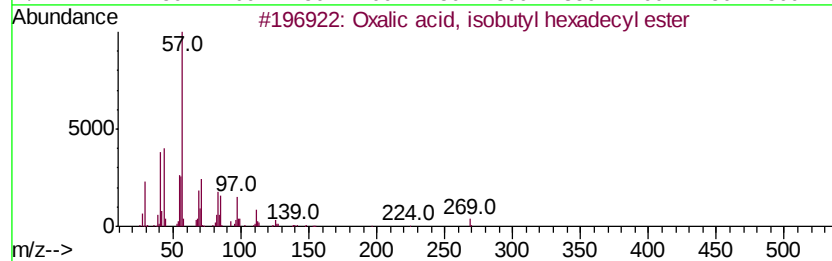
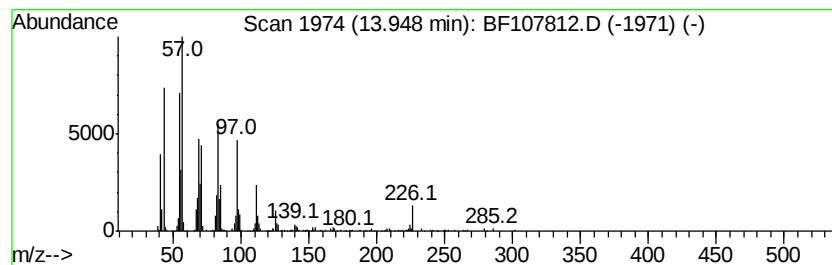
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Oxalic acid, isobutyl hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	4.53 ng	410104	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
2		Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91
3		Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	91
4		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
5		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91



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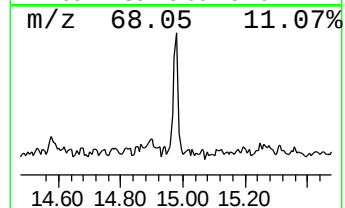
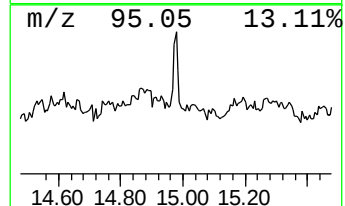
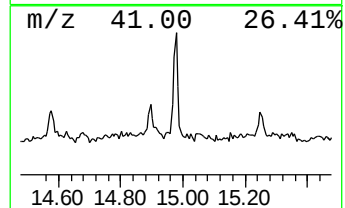
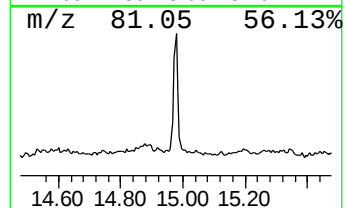
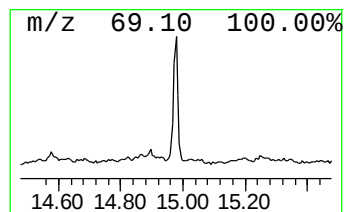
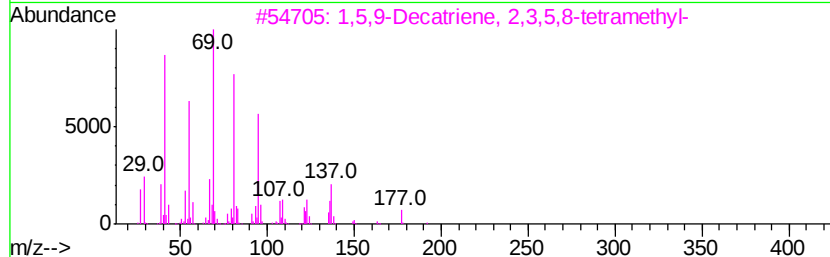
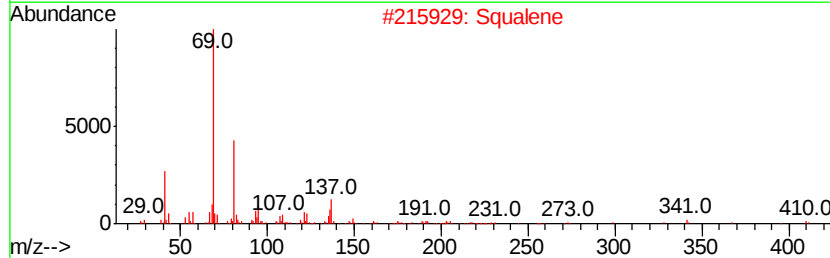
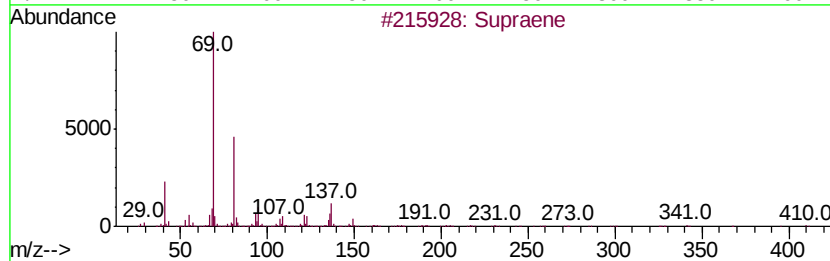
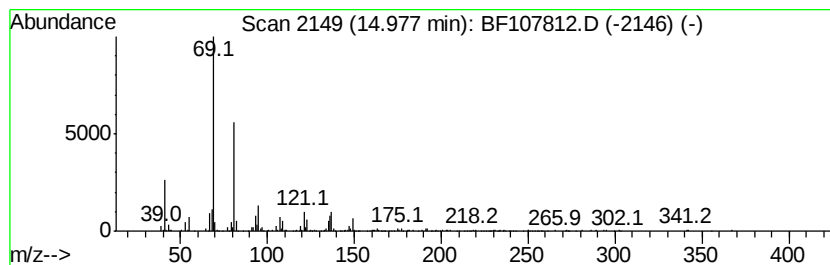
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Peak Number 5 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	3.91 ng	260401	Perylene-d12	15.68

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene		410	C30H50	007683-64-9	91
2	Squalene		410	C30H50	000111-02-4	90
3	1,5,9-Decatriene, 2,3,5,8-tetram...		192	C14H24	230646-72-7	72
4	7,11-Dimethyldodeca-2,6,10-trien...		208	C14H24O	125529-10-4	72
5	Farnesol isomer a		222	C15H26O	1000108-92-4	72



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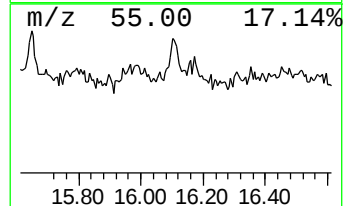
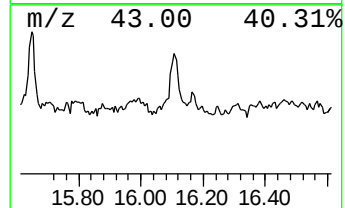
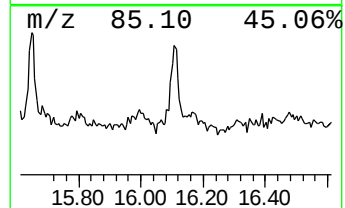
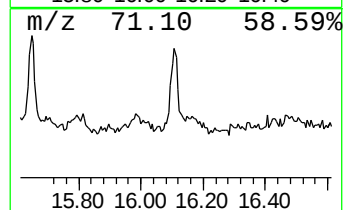
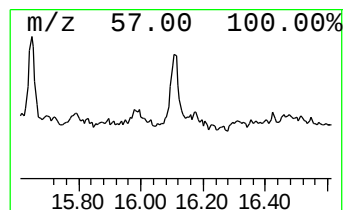
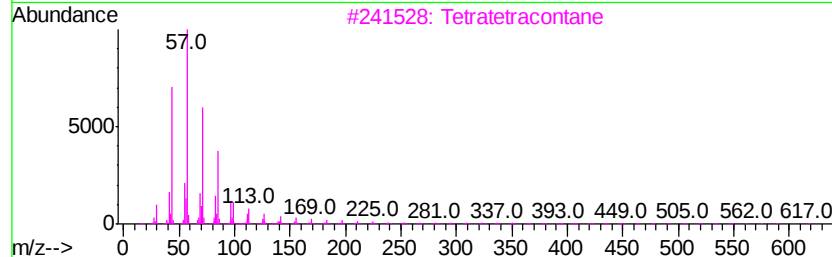
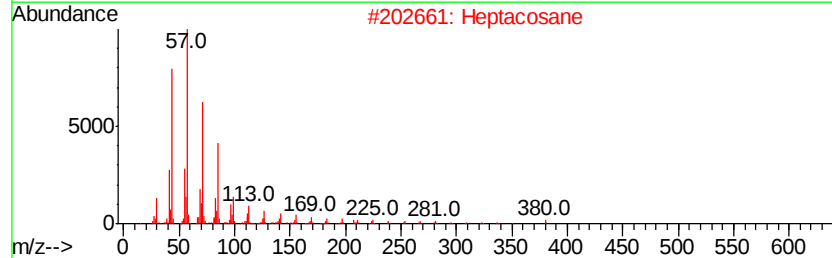
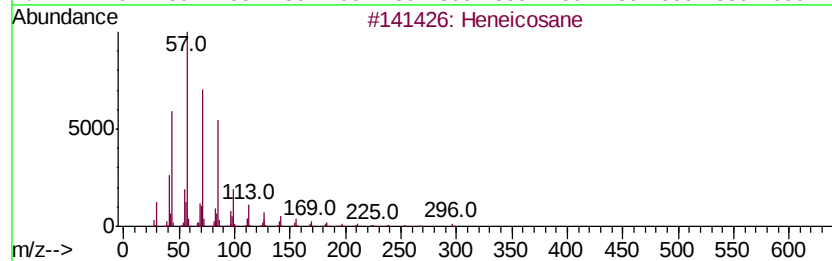
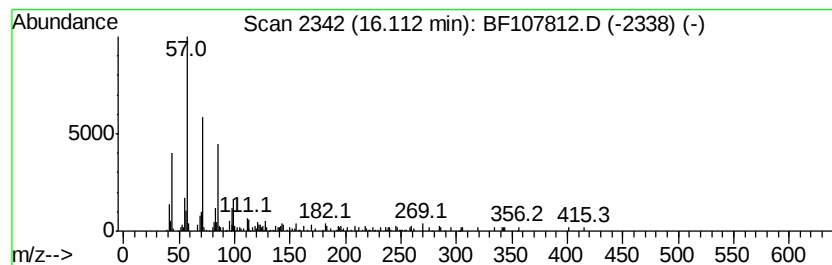
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Peak Number 6 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.11	2.11 ng	140387	Perylene-d12	15.68

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	93
2	Heptacosane		380	C27H56	000593-49-7	83
3	Tetratetracontane		619	C44H90	007098-22-8	83
4	Tetracosane		338	C24H50	000646-31-1	83
5	Docosane, 11-decyl-		451	C32H66	055401-55-3	80



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.20	14.1	ng	873807	1	6.96	1237400	20.0
unknown6.74	6.74	91.7	ng	5671890	1	6.96	1237400	20.0
Oxalic acid, isob...	13.95	4.5	ng	410104	5	14.15	1809950	20.0
Supraene	14.98	3.9	ng	260401	6	15.68	1331750	20.0
Heneicosane	16.11	2.1	ng	140387	6	15.68	1331750	20.0