

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010318\
 Data File : BF101858.D
 Acq On : 3 Jan 2018 14:29
 Operator : SJ/JU
 Sample : PB105431BL
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB105431BL

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:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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	5.016	494	498	510	rBV	117950	248280	6.63%	0.815%
2	5.398	560	563	598	rBV	2513404	3631179	96.96%	11.915%
3	6.416	733	736	754	rBV	2465328	3417173	91.24%	11.213%
4	6.545	754	758	773	rVB	3020996	3289271	87.83%	10.793%
5	6.769	793	796	807	rBV	728461	748218	19.98%	2.455%
6	6.922	818	822	839	rBV	2516258	2739766	73.16%	8.990%
7	7.339	890	893	915	rBV	1801501	2282080	60.94%	7.488%
8	8.051	1011	1014	1033	rBV	896251	1007072	26.89%	3.305%
9	9.122	1191	1196	1212	rBV	3541361	3745101	100.00%	12.289%
10	9.804	1308	1312	1325	rVB	1094714	1080148	28.84%	3.544%
11	10.604	1444	1448	1466	rBV	1843541	2155673	57.56%	7.074%
12	11.298	1562	1566	1577	rBV	1071452	1106510	29.55%	3.631%
13	11.804	1648	1652	1662	rBV2	78449	121465	3.24%	0.399%
14	12.592	1782	1786	1794	rBV	74971	106077	2.83%	0.348%
15	12.874	1830	1834	1838	rBV	2967938	3130611	83.59%	10.273%
16	13.798	1987	1991	1997	rBV	35667	42851	1.14%	0.141%
17	13.951	2013	2017	2026	rBV	713590	825786	22.05%	2.710%
18	14.327	2071	2081	2086	rBV10	17219	59637	1.59%	0.196%
19	14.739	2147	2151	2156	rVB	55558	70326	1.88%	0.231%
20	15.415	2261	2266	2281	rVB	401425	668039	17.84%	2.192%

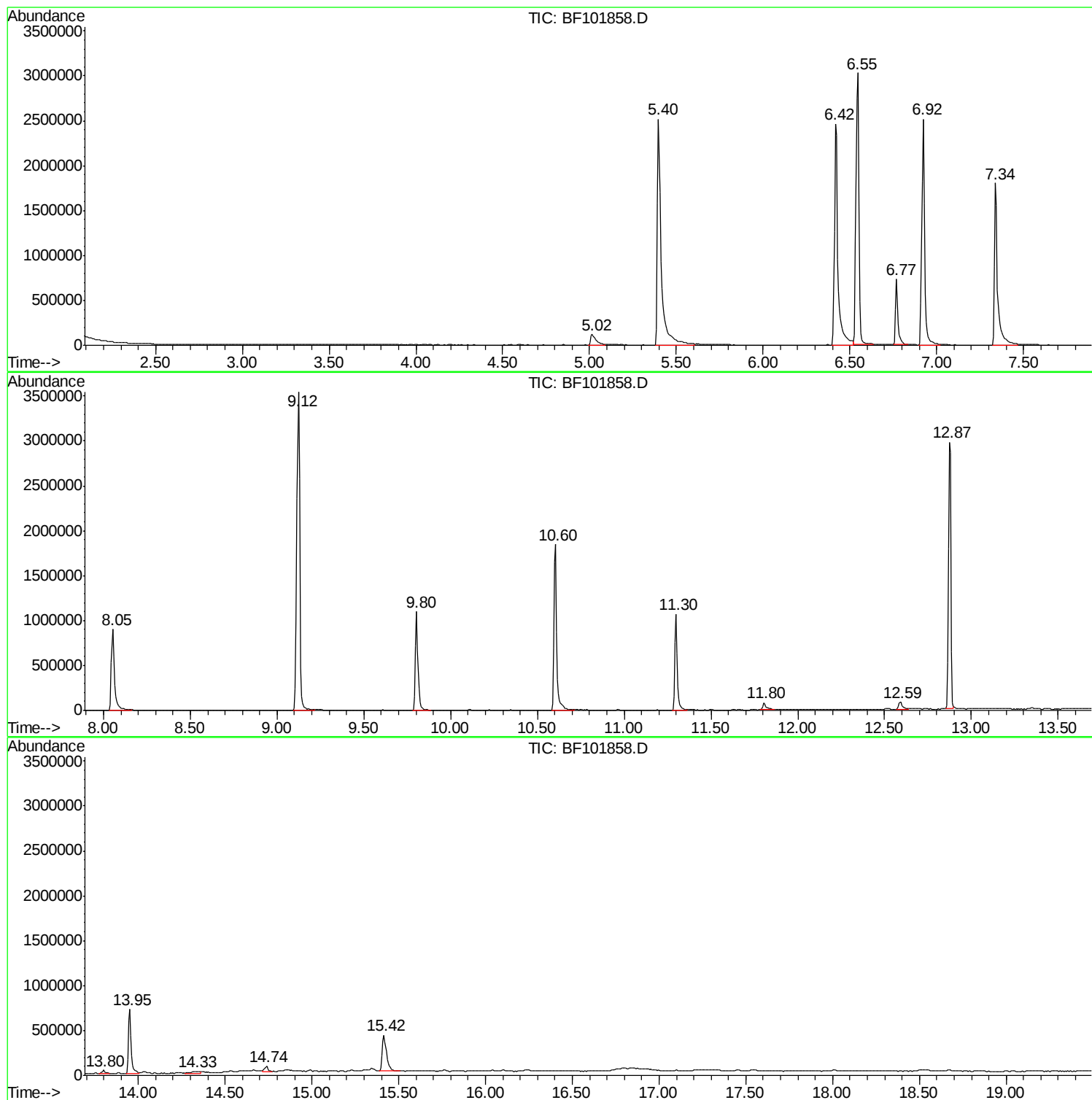
Sum of corrected areas: 30475263

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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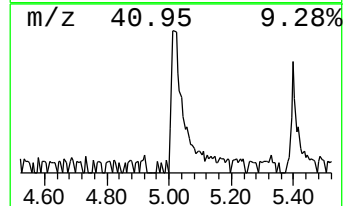
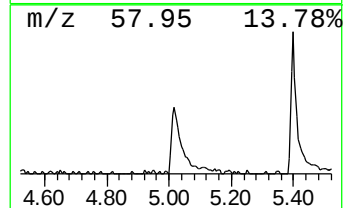
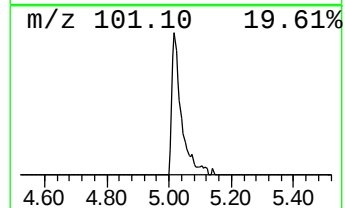
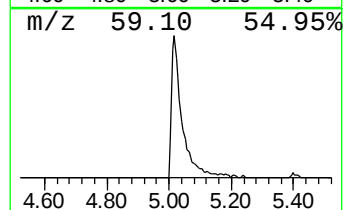
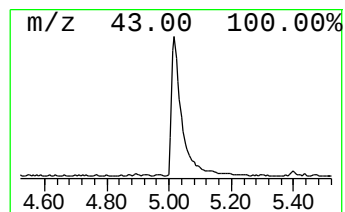
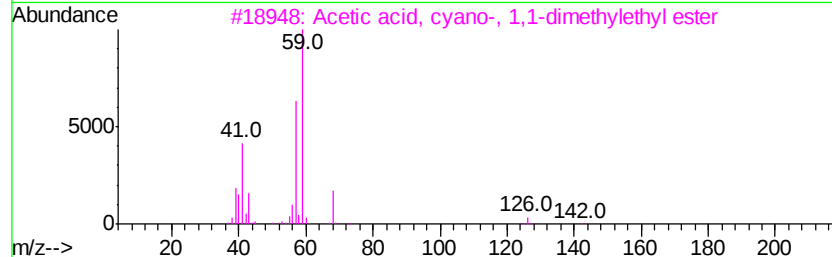
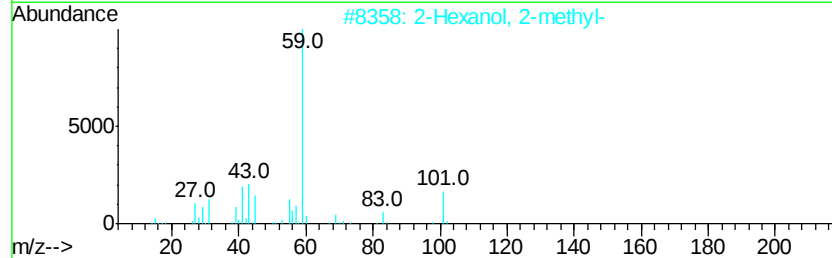
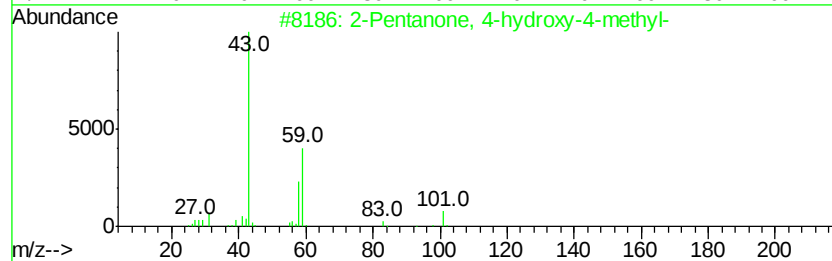
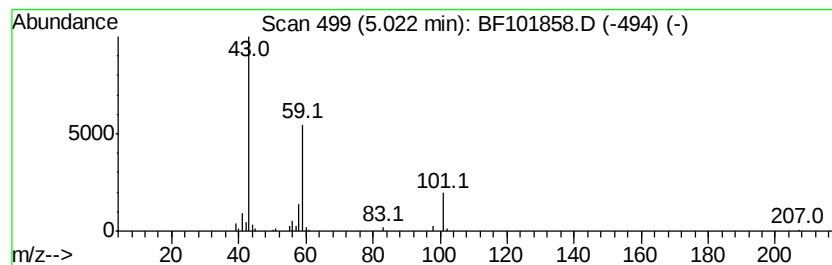
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.02	6.64 ng	248280	1,4-Dichlorobenzene-d4	6.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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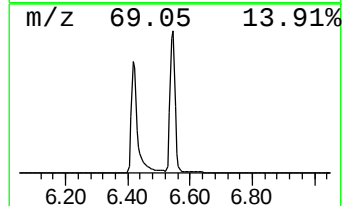
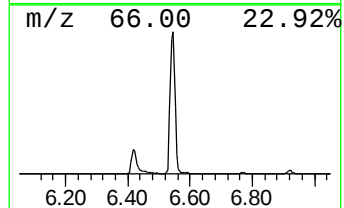
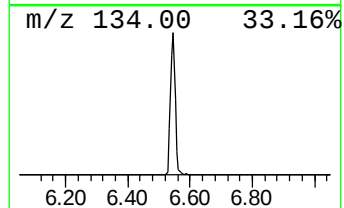
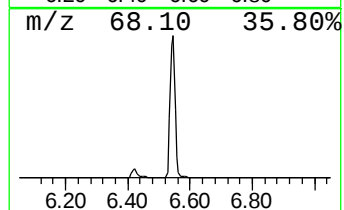
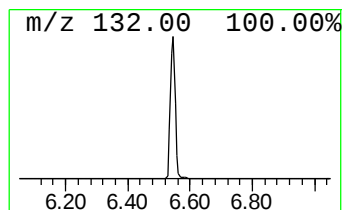
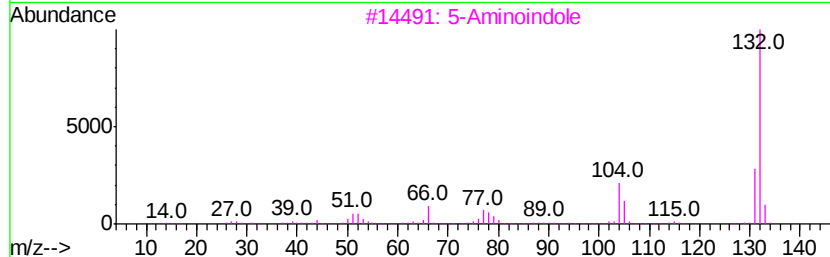
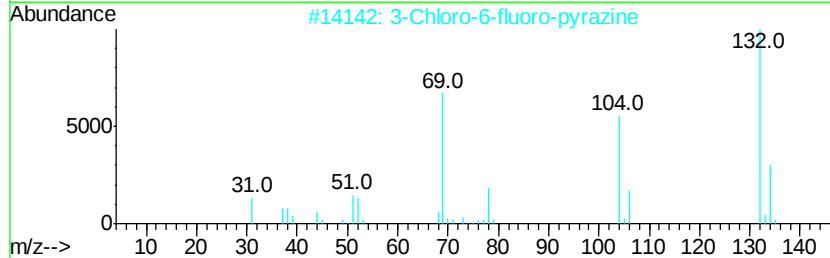
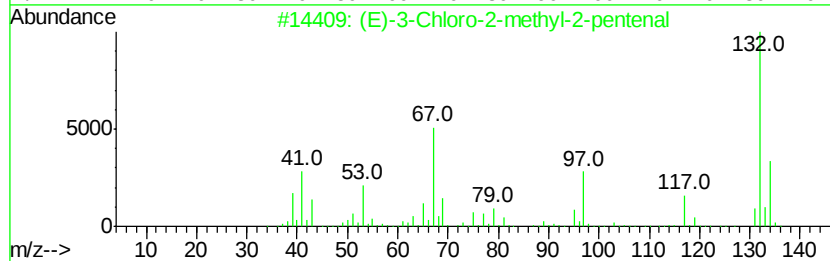
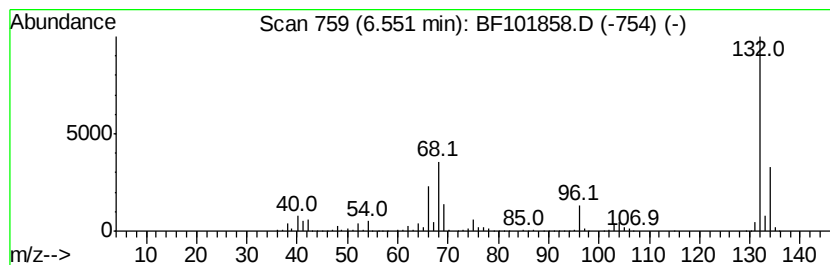
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Peak Number 2 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	87.92 ng	3289270	1,4-Dichlorobenzene-d4	6.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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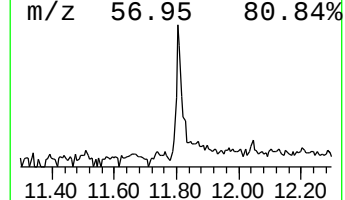
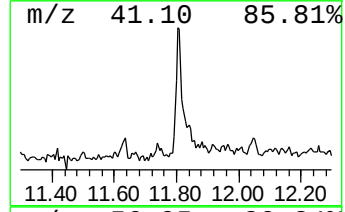
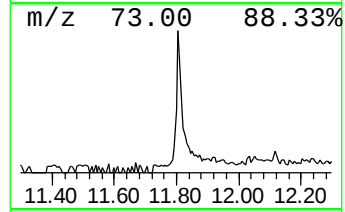
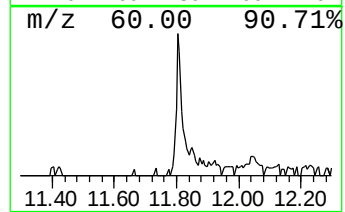
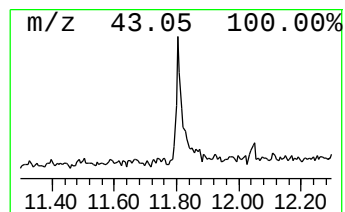
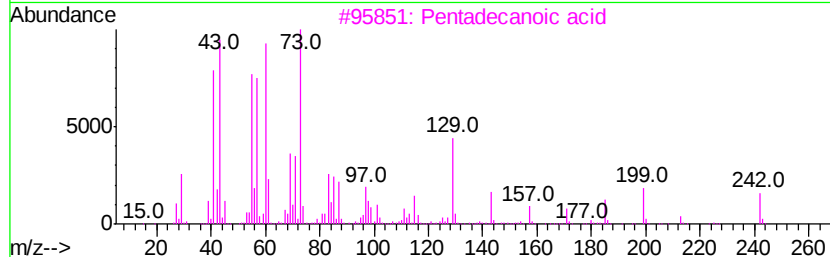
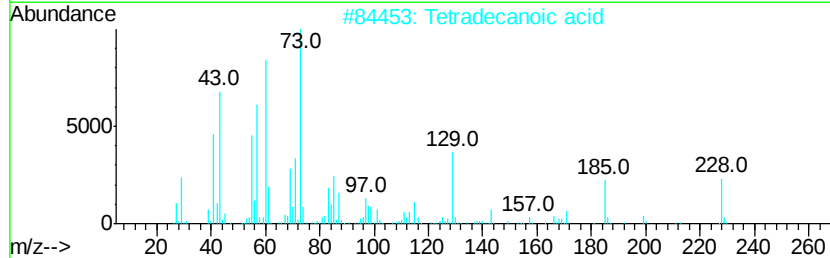
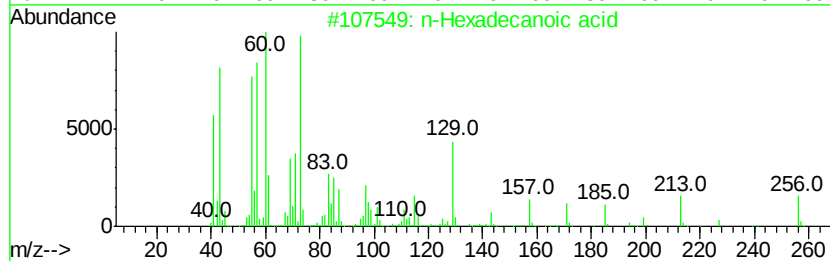
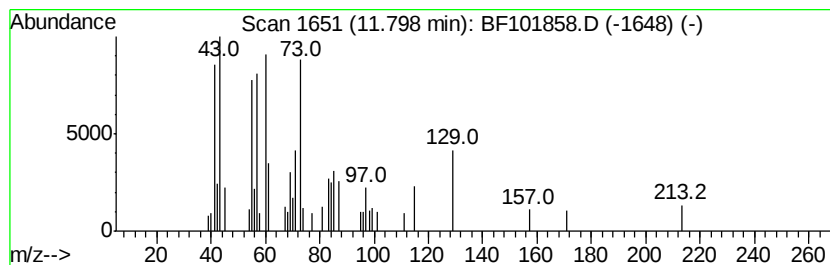
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.80	2.20 ng	121465	Phenanthrene-d10	11.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	59
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4		Tridecanoic acid	214	C13H26O2	000638-53-9	53
5		Oxalic acid, dodecyl isobutyl ester	314	C18H34O4	1000309-37-7	22



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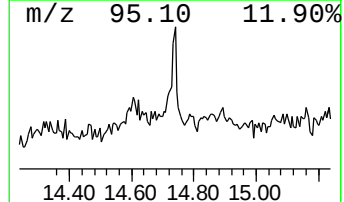
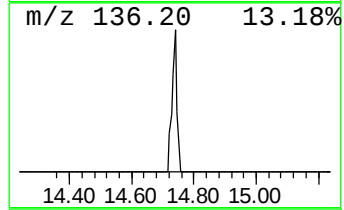
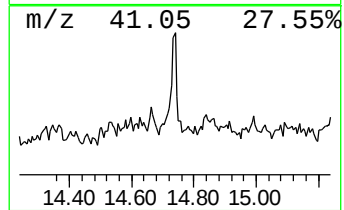
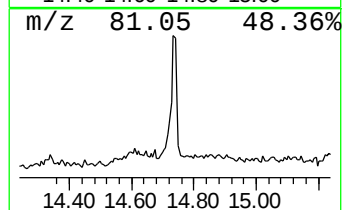
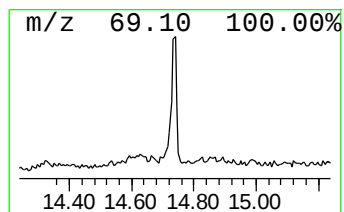
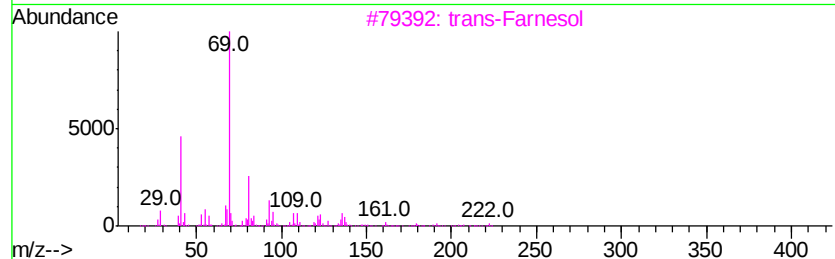
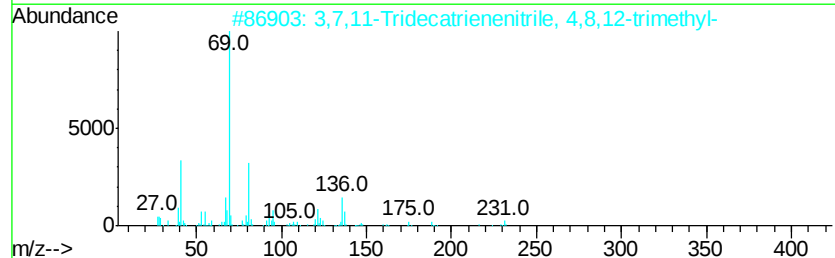
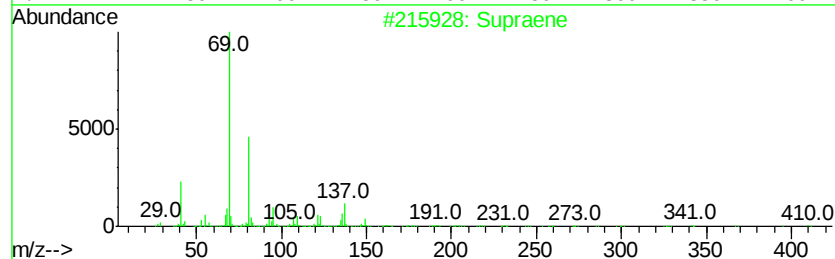
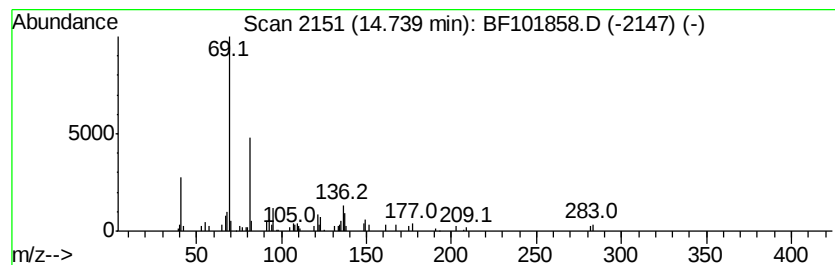
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Peak Number 5 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.74	2.11 ng	70326	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	72
2		3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	64
3		trans-Farnesol	222	C15H26O	000106-28-5	64
4		Squalene	410	C30H50	000111-02-4	64
5		2,7,11-Trimethyl-4-phenylthiodod...	314	C21H30S	1000190-11-3	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.02	6.6	ng	248280	1	6.77	748218	20.0
unknown6.55	6.55	87.9	ng	3289270	1	6.77	748218	20.0
n-Hexadecanoic acid	11.80	2.2	ng	121465	4	11.30	1106510	20.0
Supraene	14.74	2.1	ng	70326	6	15.42	668039	20.0