

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121618\
 Data File : BF111520.D
 Acq On : 16 Dec 2018 20:47
 Operator : JU/SJ
 Sample : J6340-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-02A

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-BF121418.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	4.999	488	495	504	rBV	170912	224856	3.81%	0.515%
2	5.422	562	567	570	rBV	3963967	3844808	65.14%	8.803%
3	6.440	735	740	757	rBV	5394375	5902347	100.00%	13.514%
4	6.563	757	761	765	rBV	5582124	5492558	93.06%	12.575%
5	6.787	796	799	803	rBV	1456949	1167074	19.77%	2.672%
6	6.945	822	826	829	rBV	4796827	4357825	73.83%	9.977%
7	7.351	889	895	898	rBV	3594031	3567318	60.44%	8.167%
8	8.069	1013	1017	1037	rBV	1723865	1543969	26.16%	3.535%
9	9.145	1195	1200	1204	rBV	5955150	5850755	99.13%	13.395%
10	9.534	1263	1266	1274	rVB	319603	307969	5.22%	0.705%
11	9.822	1311	1315	1331	rVB2	1586507	1466762	24.85%	3.358%
12	10.610	1445	1449	1458	rBV	2517363	2370611	40.16%	5.428%
13	11.304	1563	1567	1574	rBV	1214777	1135100	19.23%	2.599%
14	11.839	1654	1658	1666	rBV3	98067	141205	2.39%	0.323%
15	12.516	1770	1773	1776	rBV	79478	75960	1.29%	0.174%
16	12.892	1833	1837	1840	rBV	4369809	3919397	66.40%	8.974%
17	13.798	1987	1991	1998	rVB2	151407	215756	3.66%	0.494%
18	13.945	2011	2016	2019	rBV	1127133	1218509	20.64%	2.790%
19	14.792	2157	2160	2164	rVB	125400	120430	2.04%	0.276%
20	15.380	2256	2260	2264	rBV	650724	753952	12.77%	1.726%

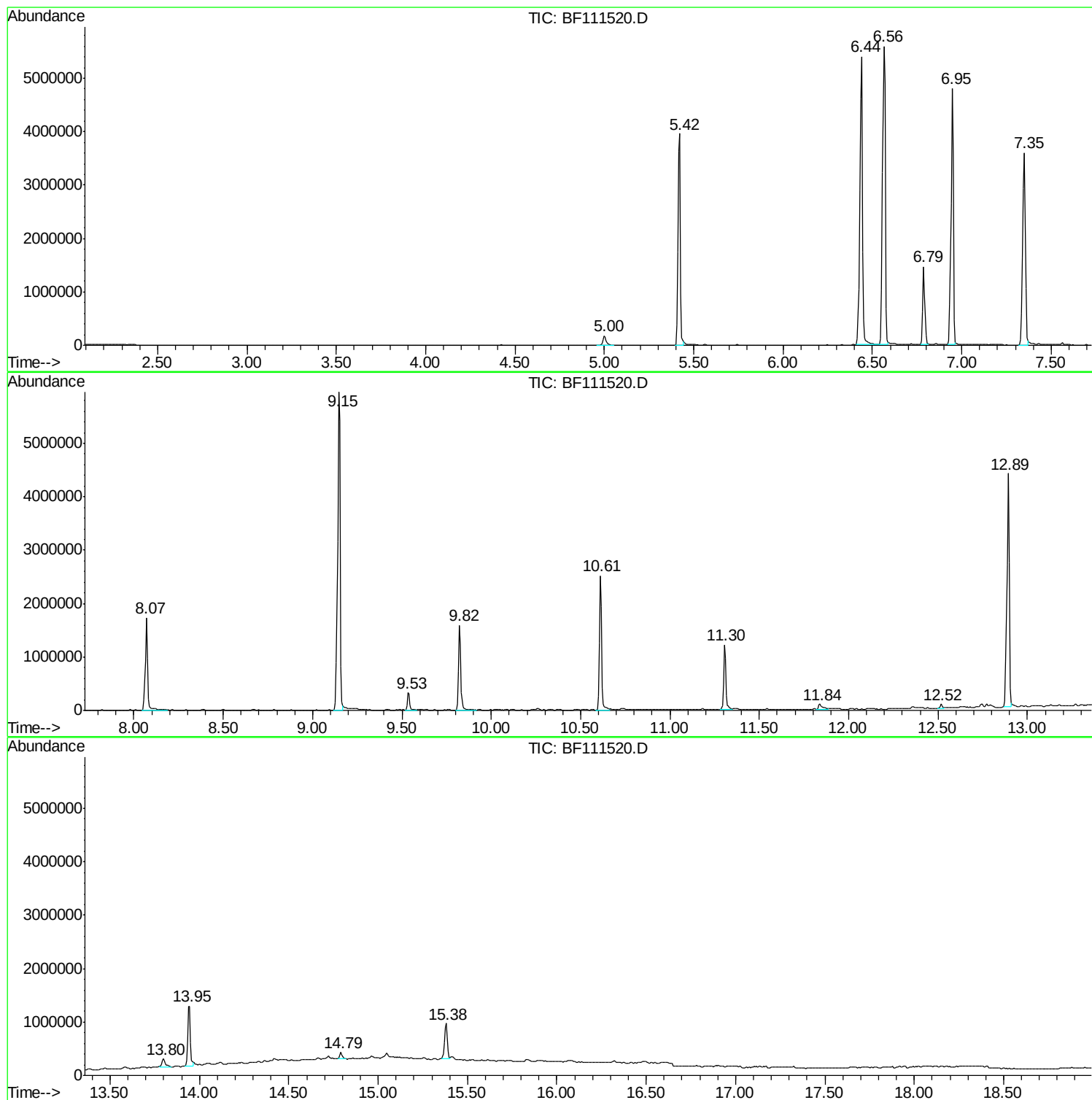
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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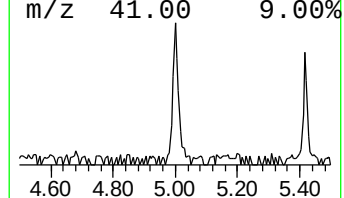
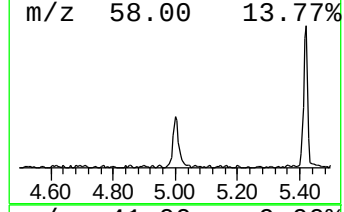
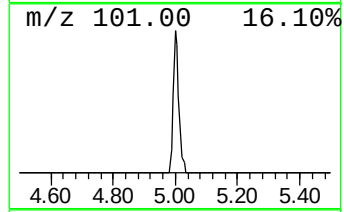
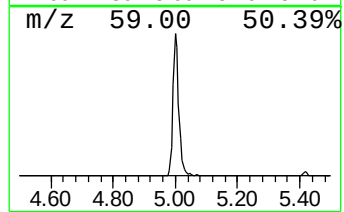
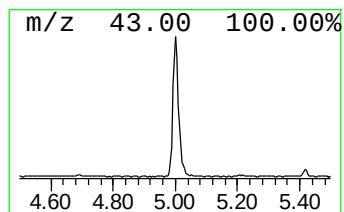
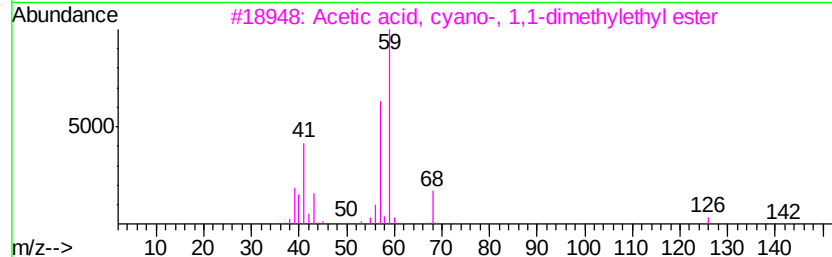
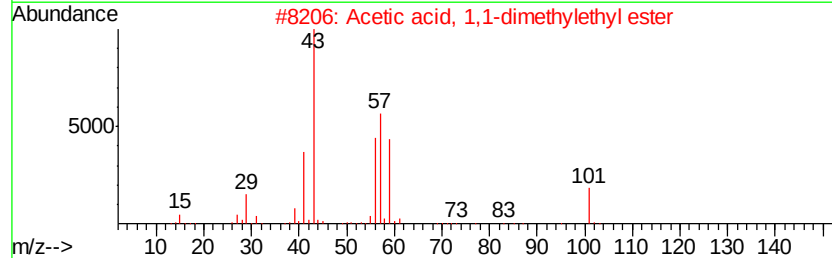
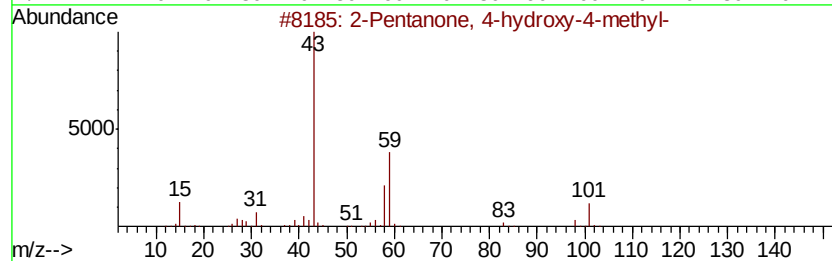
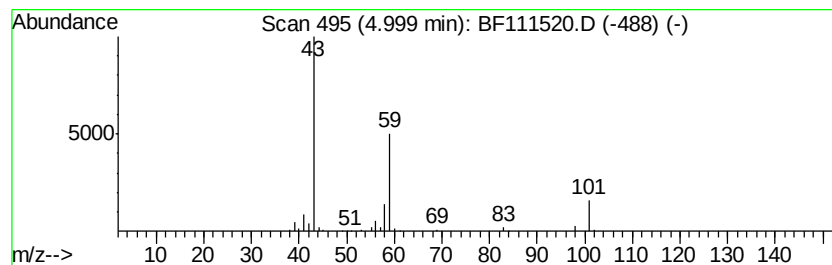
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.00	3.85 ng	224856	1,4-Dichlorobenzene-d4	6.79

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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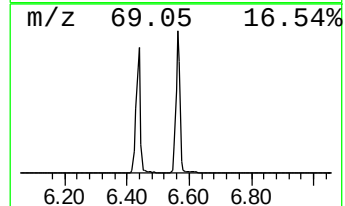
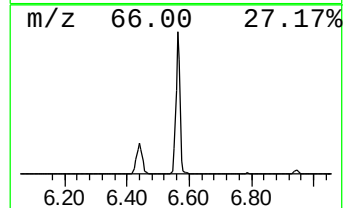
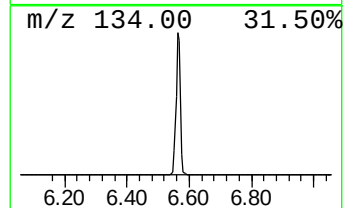
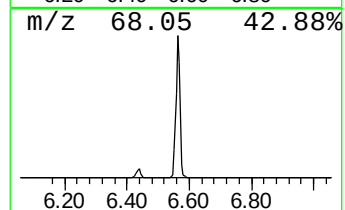
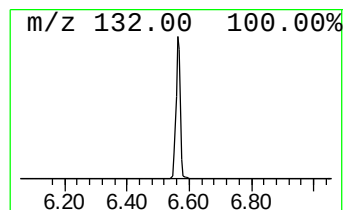
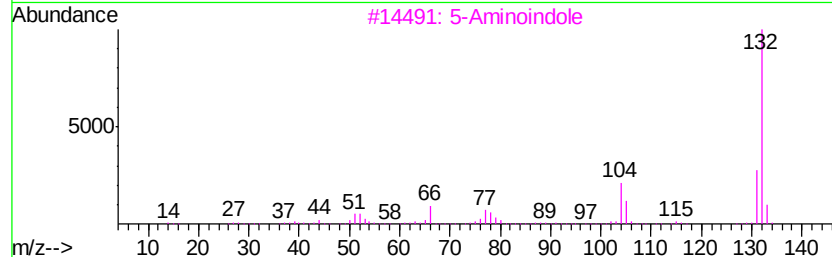
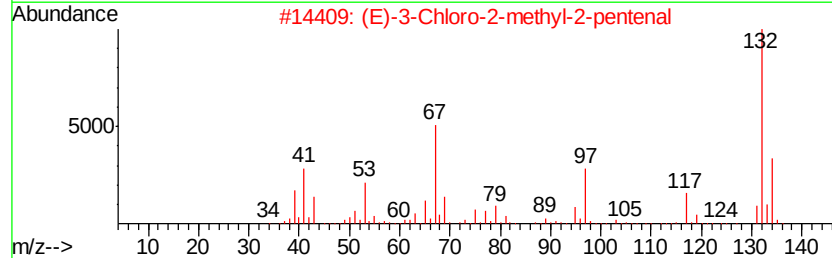
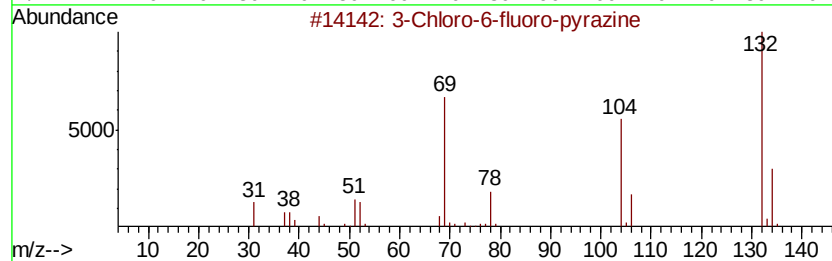
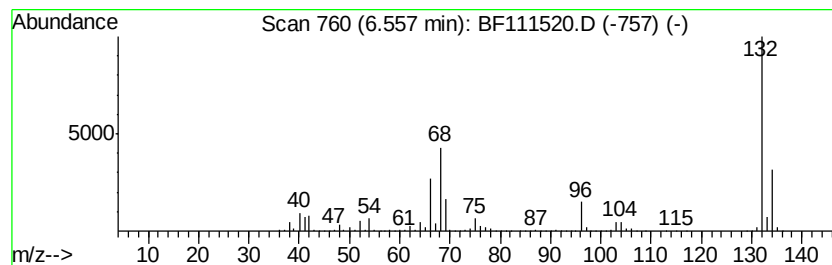
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Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	94.13 ng	5492560	1,4-Dichlorobenzene-d4	6.79

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-Aminoindole	132	C8H8N2	005192-03-0	12
4		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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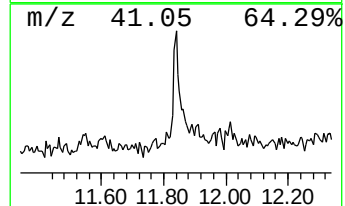
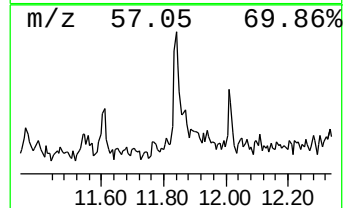
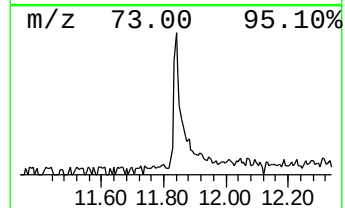
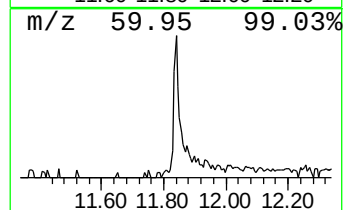
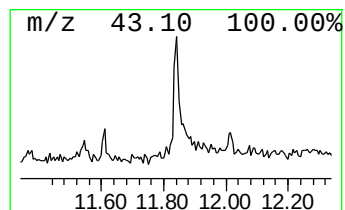
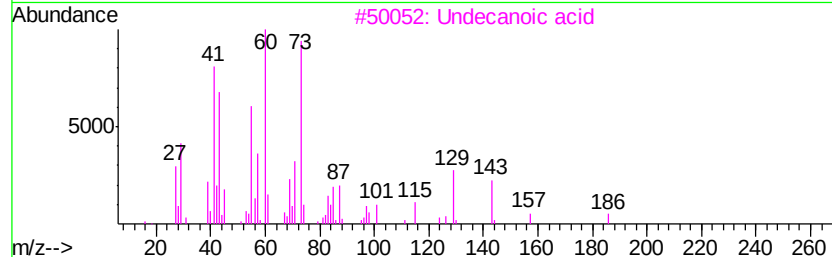
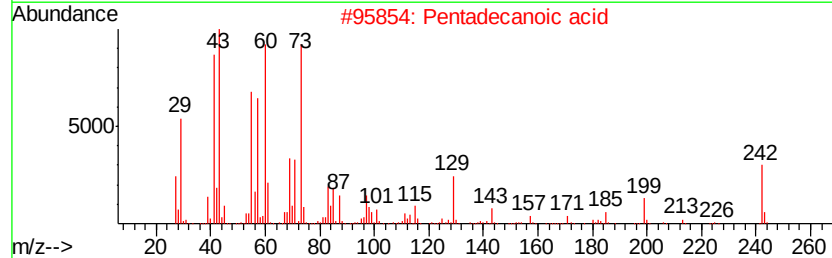
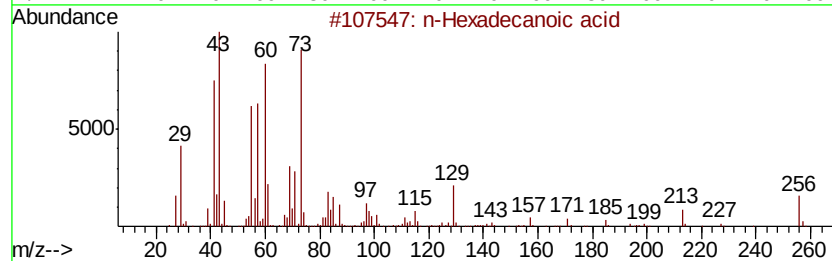
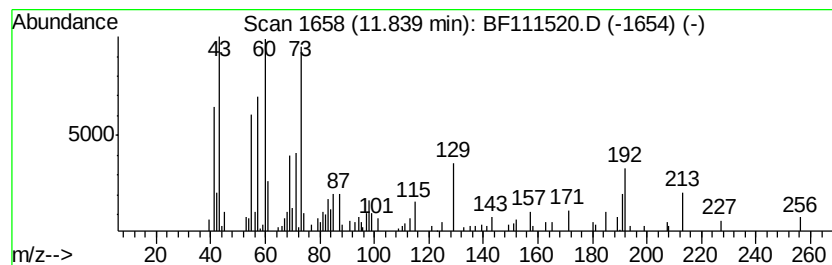
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.84	2.49 ng	141205	Phenanthrene-d10		11.30
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	Undecanoic acid	186	C11H22O2	000112-37-8	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Tridecanoic acid	214	C13H26O2	000638-53-9	52



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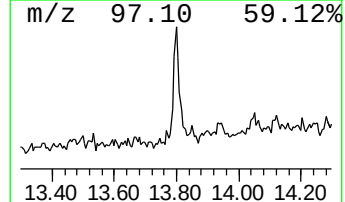
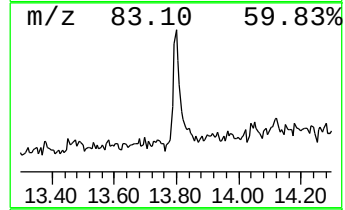
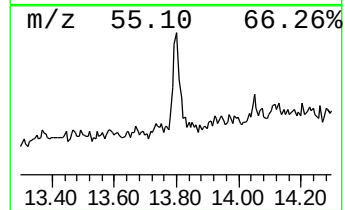
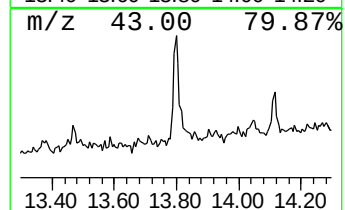
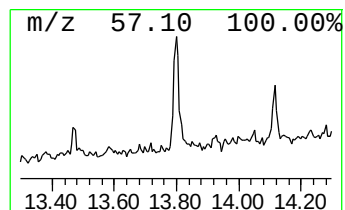
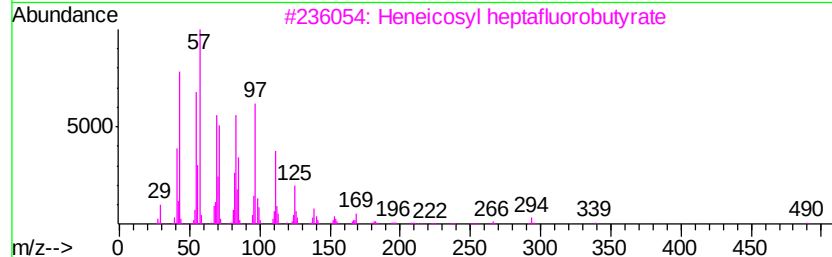
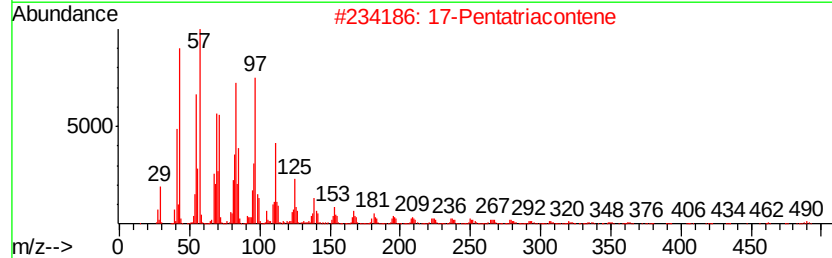
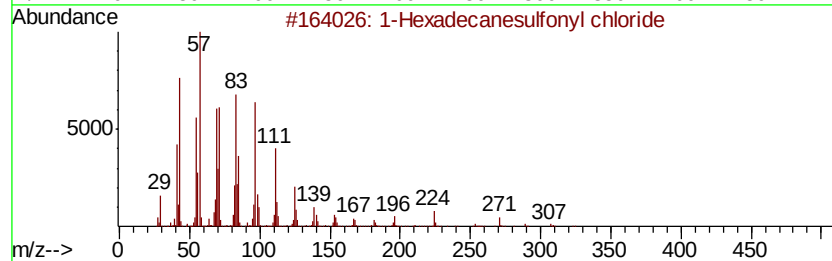
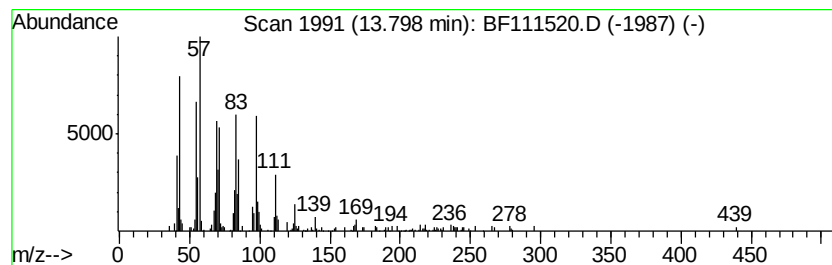
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 1-Hexadecanesulfonyl chloride Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.80	3.54 ng	215756	Chrysene-d12	13.95		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
2		17-Pentatriacontene	491	C35H70	006971-40-0	91
3		Heneicosyl heptafluorobutyrat	508	C25H43F7O2	1000351-83-8	91
4		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
5		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90



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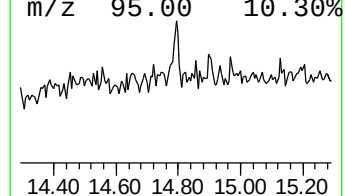
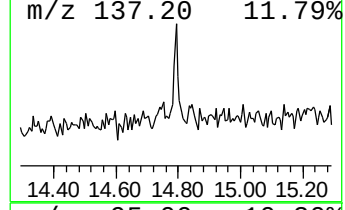
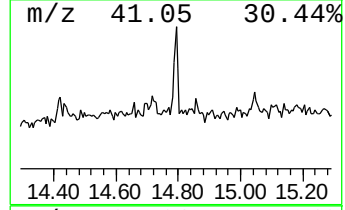
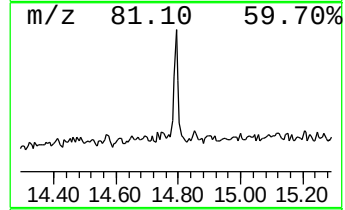
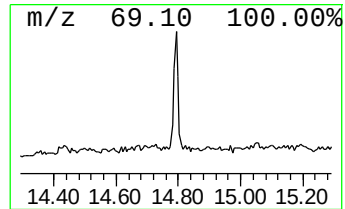
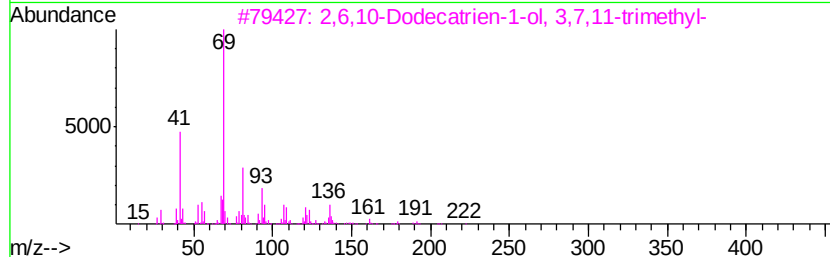
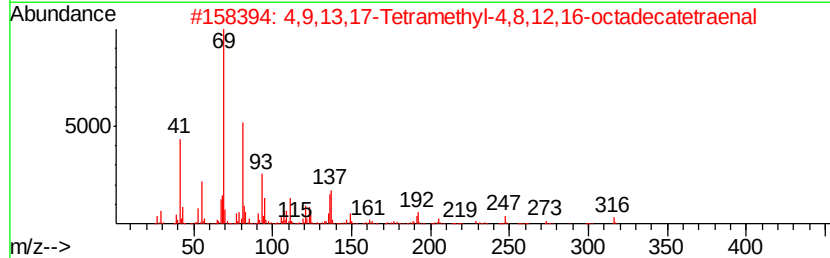
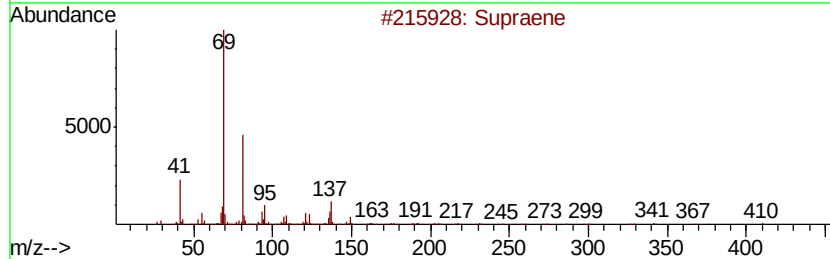
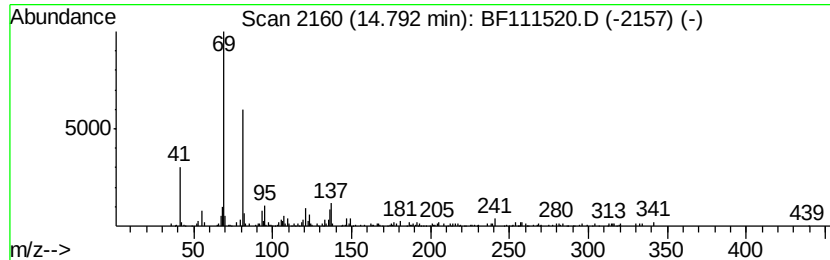
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	3.19 ng	120430	Perylene-d12	15.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	83
2		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	80
3		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72
4		Squalene	410	C30H50	000111-02-4	72
5		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.00	3.9	ng	224856	1	6.79	1167070	20.0
unknown6.56	6.56	94.1	ng	5492560	1	6.79	1167070	20.0
n-Hexadecanoic acid	11.84	2.5	ng	141205	4	11.30	1135100	20.0
1-Hexadecanesulfo...	13.80	3.5	ng	215756	5	13.95	1218510	20.0
Supraene	14.79	3.2	ng	120430	6	15.38	753952	20.0