

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072717\
 Data File : BF097132.D
 Acq On : 27 Jul 2017 19:45
 Operator : SJ/JU
 Sample : I4424-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 AU-06-072417-A

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:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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	3.210	218	225	232	rBV	39646	79214	3.77%	0.451%
2	4.628	462	466	484	rVB	220842	324414	15.45%	1.846%
3	5.087	540	544	557	rBV	2039910	2100356	100.00%	11.950%
4	6.151	720	725	735	rBV	1766977	1904012	90.65%	10.833%
5	6.257	739	743	754	rVB	2052416	1806685	86.02%	10.279%
6	6.487	778	782	791	rVB	638057	551623	26.26%	3.138%
7	6.639	804	808	819	rBV	1447641	1340316	63.81%	7.626%
8	7.051	874	878	891	rBV	1305988	1194012	56.85%	6.793%
9	7.769	996	1000	1008	rBV	776645	658574	31.36%	3.747%
10	8.845	1179	1183	1186	rBV	1733171	1461986	69.61%	8.318%
11	9.245	1247	1251	1256	rBV	238210	186312	8.87%	1.060%
12	9.510	1293	1296	1301	rBV	623522	588484	28.02%	3.348%
13	9.969	1371	1374	1377	rBV	32091	27123	1.29%	0.154%
14	10.298	1426	1430	1440	rVB	927618	818131	38.95%	4.655%
15	10.439	1451	1454	1460	rBV	32610	42069	2.00%	0.239%
16	10.886	1526	1530	1532	rBV2	21602	24078	1.15%	0.137%
17	10.986	1543	1547	1550	rBV	568384	479024	22.81%	2.725%
18	11.404	1615	1618	1622	rBV	158891	139111	6.62%	0.791%
19	11.539	1639	1641	1649	rBV2	40708	46499	2.21%	0.265%
20	12.086	1730	1734	1736	rBV	566224	519049	24.71%	2.953%
21	12.104	1736	1737	1746	rVB	362414	309700	14.75%	1.762%
22	12.192	1748	1752	1755	rBV	126856	110521	5.26%	0.629%
23	12.416	1786	1790	1797	rBV2	55161	68463	3.26%	0.390%
24	12.569	1812	1816	1820	rVB	1343661	1186778	56.50%	6.752%
25	13.480	1968	1971	1978	rVB3	63825	74948	3.57%	0.426%
26	13.610	1989	1993	1996	rBV	624224	573639	27.31%	3.264%
27	13.721	2007	2012	2014	rBV4	16852	27144	1.29%	0.154%
28	14.110	2076	2078	2082	rBV4	22174	30460	1.45%	0.173%
29	14.139	2082	2083	2087	rBV4	29097	39410	1.88%	0.224%
30	14.663	2170	2172	2174	rBV3	29274	32909	1.57%	0.187%
31	14.957	2218	2222	2228	rVB	406268	462822	22.04%	2.633%
32	15.033	2232	2235	2236	rBV2	34394	35564	1.69%	0.202%
33	15.486	2309	2312	2315	rBV4	43328	46020	2.19%	0.262%
34	15.815	2366	2368	2376	rBV9	44606	89938	4.28%	0.512%

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35	16.092	2412	2415	2419	rBV6	37069	62090	2.96%	0.353%
36	16.633	2502	2507	2508	rBV5	46874	73033	3.48%	0.416%
37	17.480	2649	2651	2657	rVB7	36371	36818	1.75%	0.209%
38	19.092	2923	2925	2926	rBV2	25519	25167	1.20%	0.143%

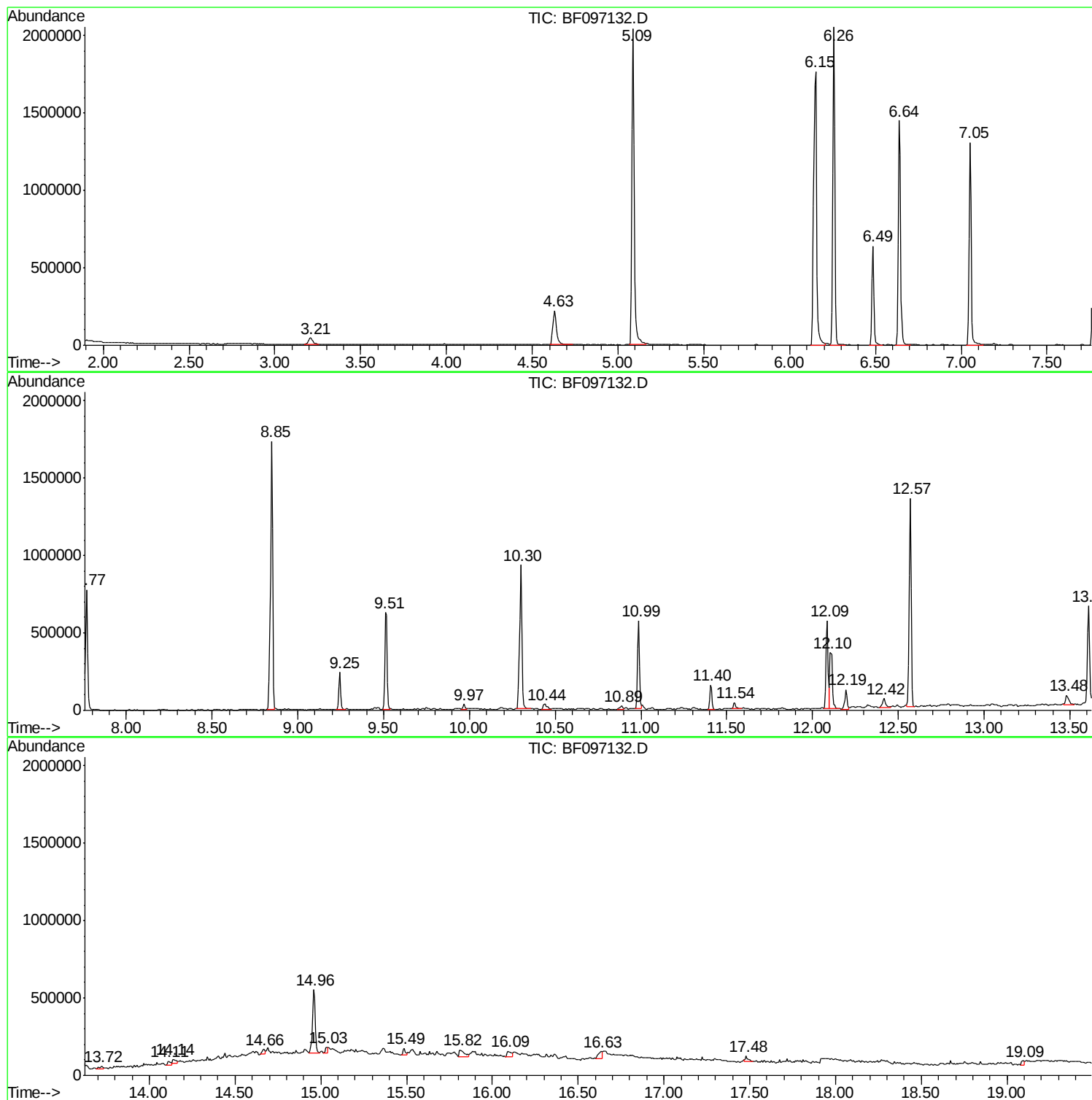
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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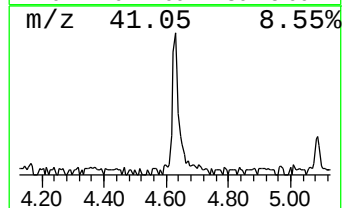
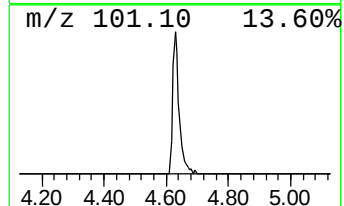
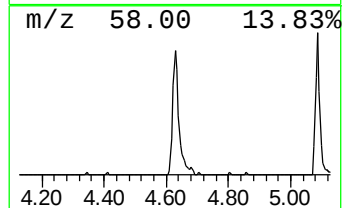
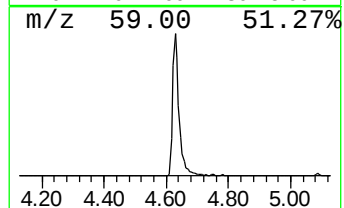
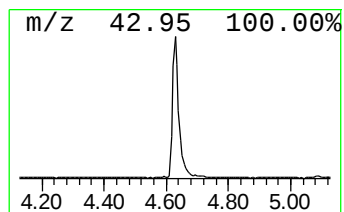
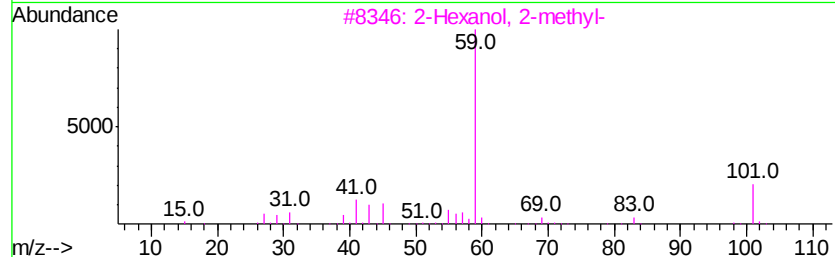
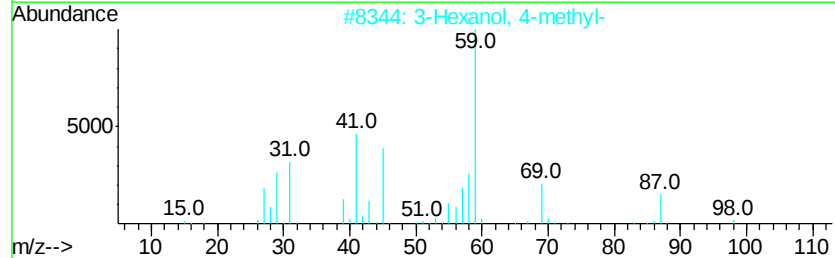
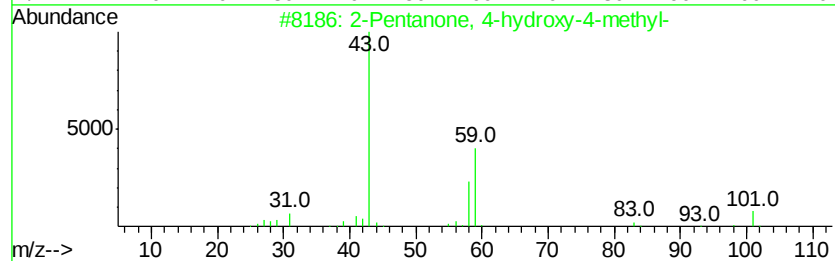
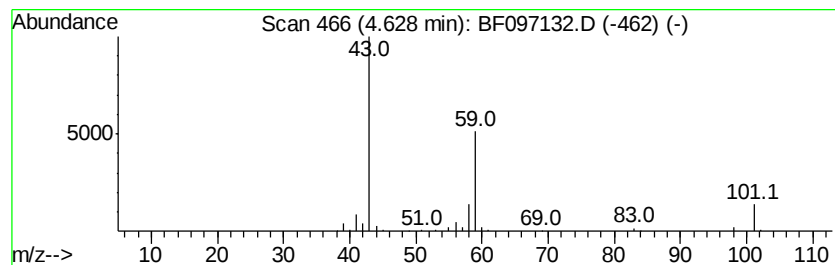
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	11.76 ng	324414	1,4-Dichlorobenzene-d4	6.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		3-Octanol	130	C8H18O	000589-98-0	33
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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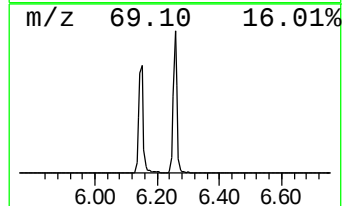
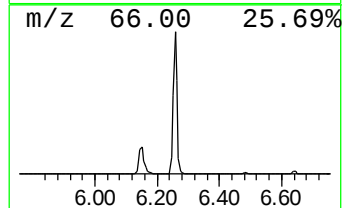
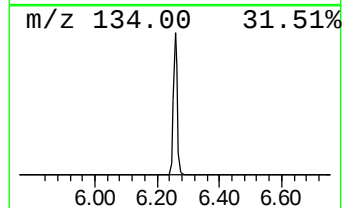
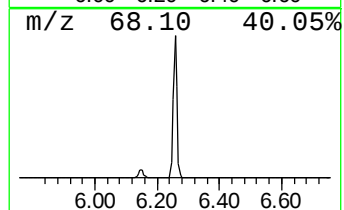
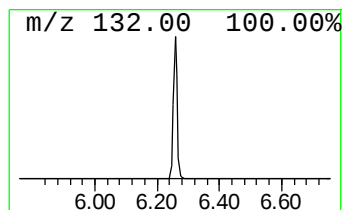
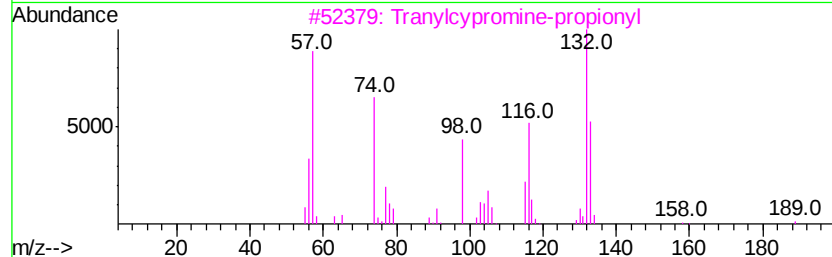
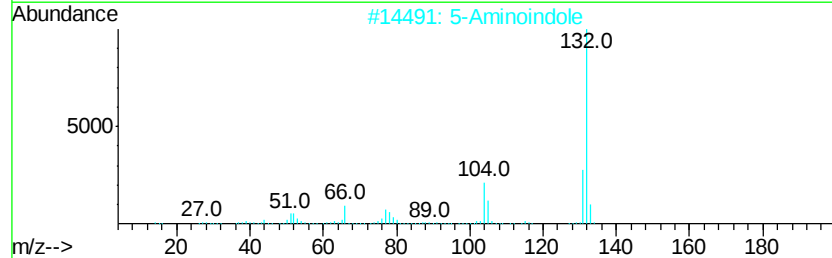
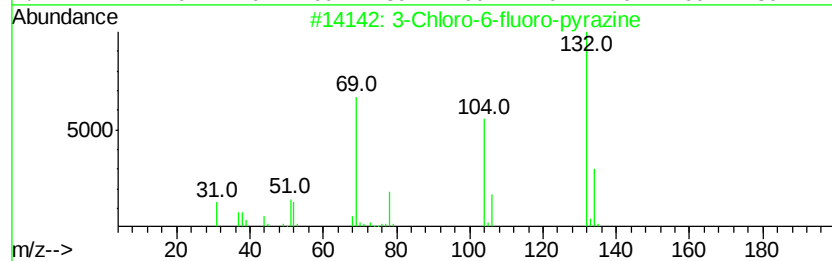
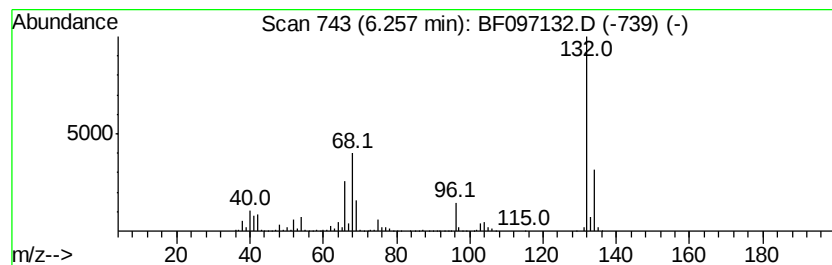
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Peak Number 3 unknown6.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.26	65.50 ng	1806690	1,4-Dichlorobenzene-d4	6.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5			4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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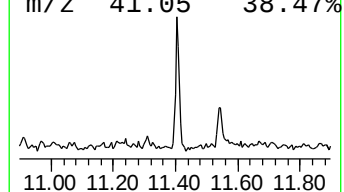
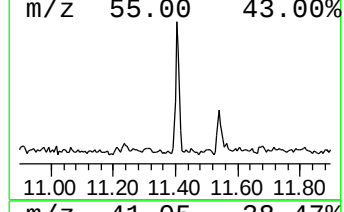
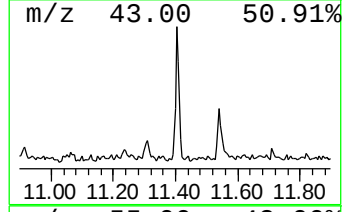
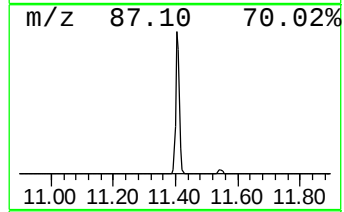
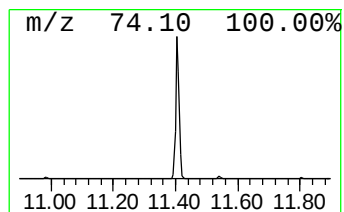
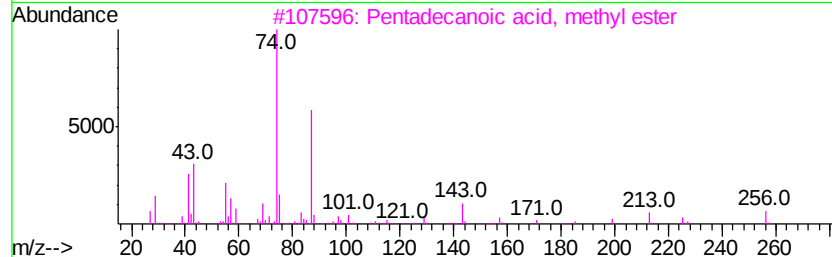
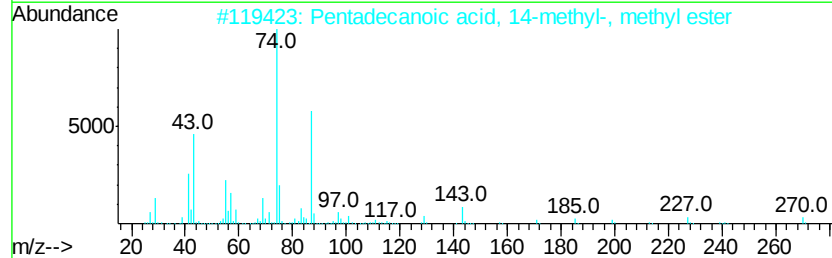
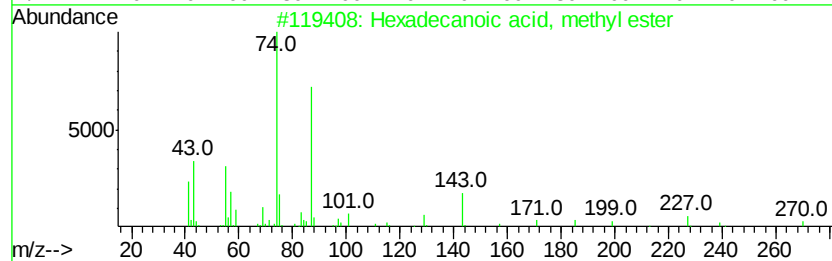
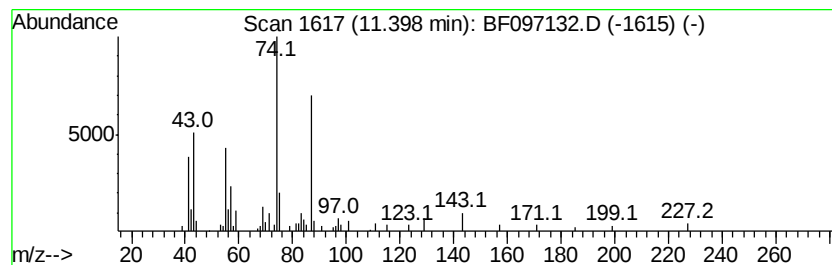
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Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.40	5.81 ng	139111	Phenanthrene-d10	10.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	91
2		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
3		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4		Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	87
5		Methyl tetradecanoate	242	C15H30O2	000124-10-7	87



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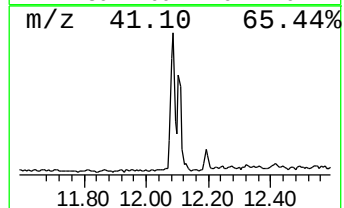
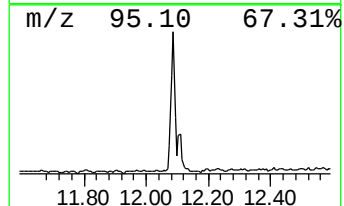
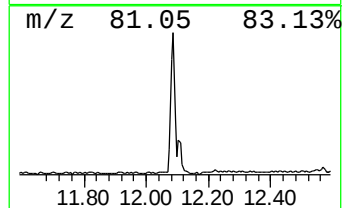
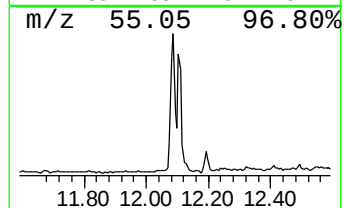
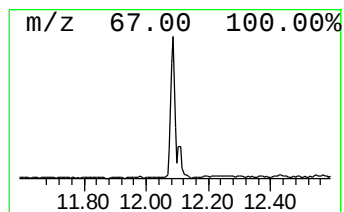
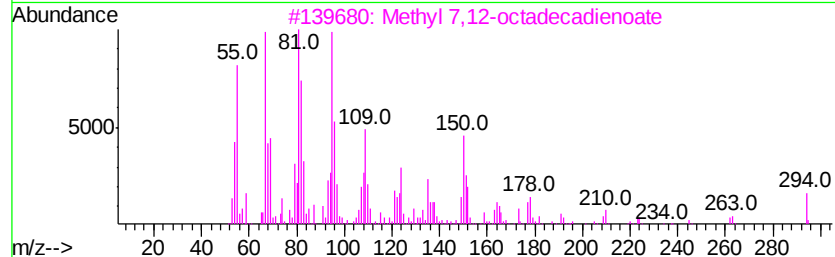
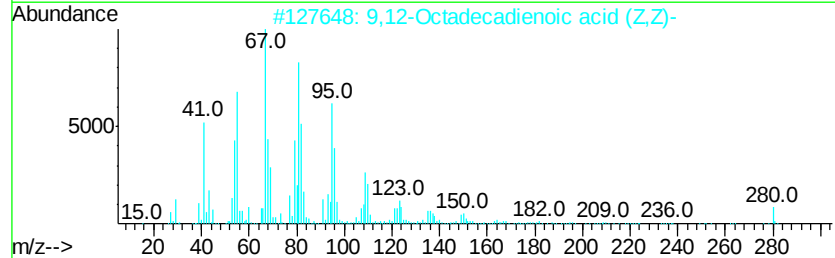
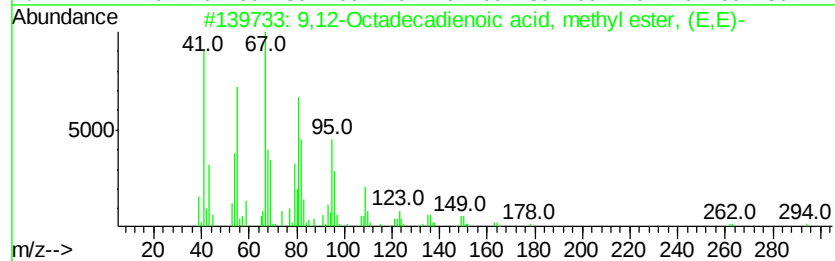
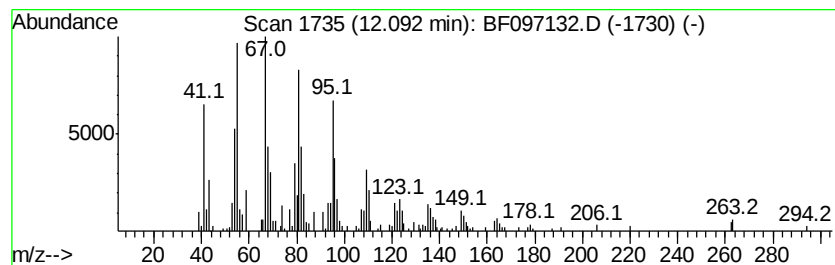
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Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.09	21.67 ng	519049	Phenanthrene-d10	10.99	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	98
2	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	95
3	Methyl 7,12-octadecadienoate	294	C19H34O2	1000336-43-8	94
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	94
5	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	93



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Peak Number 7 13-Octadecenoic acid, methy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.10	12.93 ng	309700	Phenanthrene-d10	10.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91
2		9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	90
3		9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	90
4		Methyl 12-hydroxy-9-octadecenoate	312	C19H36O3	1000336-28-8	86
5		13-Methyltetradec-9-enoic acid m...	254	C16H30O2	1000365-89-8	83

