

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
 Data File : BF107717.D
 Acq On : 26 Jul 2018 23:10
 Operator : JU/SJ
 Sample : J4109-08
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-10(10-12)

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	504	rBV	406477	711511	13.37%	1.530%
2	5.560	544	548	551	rBV	43989	66606	1.25%	0.143%
3	5.601	551	555	588	rVV	2783961	4508738	84.74%	9.697%
4	5.819	589	592	604	rVB	38242	89836	1.69%	0.193%
5	6.601	721	725	744	rBV	2889965	4587445	86.22%	9.866%
6	6.737	744	748	772	rVB	3758319	4956724	93.16%	10.661%
7	6.960	783	786	805	rBV	658751	1094839	20.58%	2.355%
8	7.119	808	813	828	rBV	2982994	3814207	71.68%	8.203%
9	7.219	828	830	837	rVB2	56053	83608	1.57%	0.180%
10	7.525	878	882	913	rBV	1993955	3249805	61.08%	6.990%
11	8.242	1000	1004	1014	rBV	1160828	1528096	28.72%	3.287%
12	9.313	1180	1186	1202	rBV	4256697	5320836	100.00%	11.444%
13	9.707	1249	1253	1265	rBV	667459	655466	12.32%	1.410%
14	10.001	1299	1303	1316	rVB	1513184	1599041	30.05%	3.439%
15	10.795	1434	1438	1451	rBV	2815975	3452420	64.88%	7.425%
16	10.883	1451	1453	1459	rVB3	43879	70436	1.32%	0.151%
17	11.495	1553	1557	1568	rBV	1293547	1626209	30.56%	3.498%
18	12.001	1639	1643	1653	rBV3	410440	518981	9.75%	1.116%
19	12.554	1733	1737	1740	rBV3	46387	64256	1.21%	0.138%
20	12.713	1760	1764	1773	rBV	239084	273709	5.14%	0.589%
21	12.942	1797	1803	1810	rBV	202922	321575	6.04%	0.692%
22	13.077	1822	1826	1837	rBV	3463827	3584379	67.36%	7.709%
23	13.271	1856	1859	1864	rVB2	56247	96451	1.81%	0.207%
24	13.954	1971	1975	1985	rVB2	411838	470765	8.85%	1.012%
25	14.142	2002	2007	2018	rBV2	1134233	1470960	27.65%	3.164%
26	14.577	2078	2081	2088	rVB3	69840	96378	1.81%	0.207%
27	14.895	2132	2135	2140	rVB	75290	79934	1.50%	0.172%
28	15.213	2186	2189	2193	rBV	98620	181077	3.40%	0.389%
29	15.248	2193	2195	2200	rVB2	124409	141224	2.65%	0.304%
30	15.542	2241	2245	2252	rVB	63610	103685	1.95%	0.223%
31	15.607	2252	2256	2260	rBV	108403	173152	3.25%	0.372%
32	15.671	2261	2267	2279	rVB	780613	1351097	25.39%	2.906%
33	16.112	2338	2342	2348	rVB	65129	95918	1.80%	0.206%
34	16.648	2429	2433	2437	rBV4	35435	56123	1.05%	0.121%

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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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

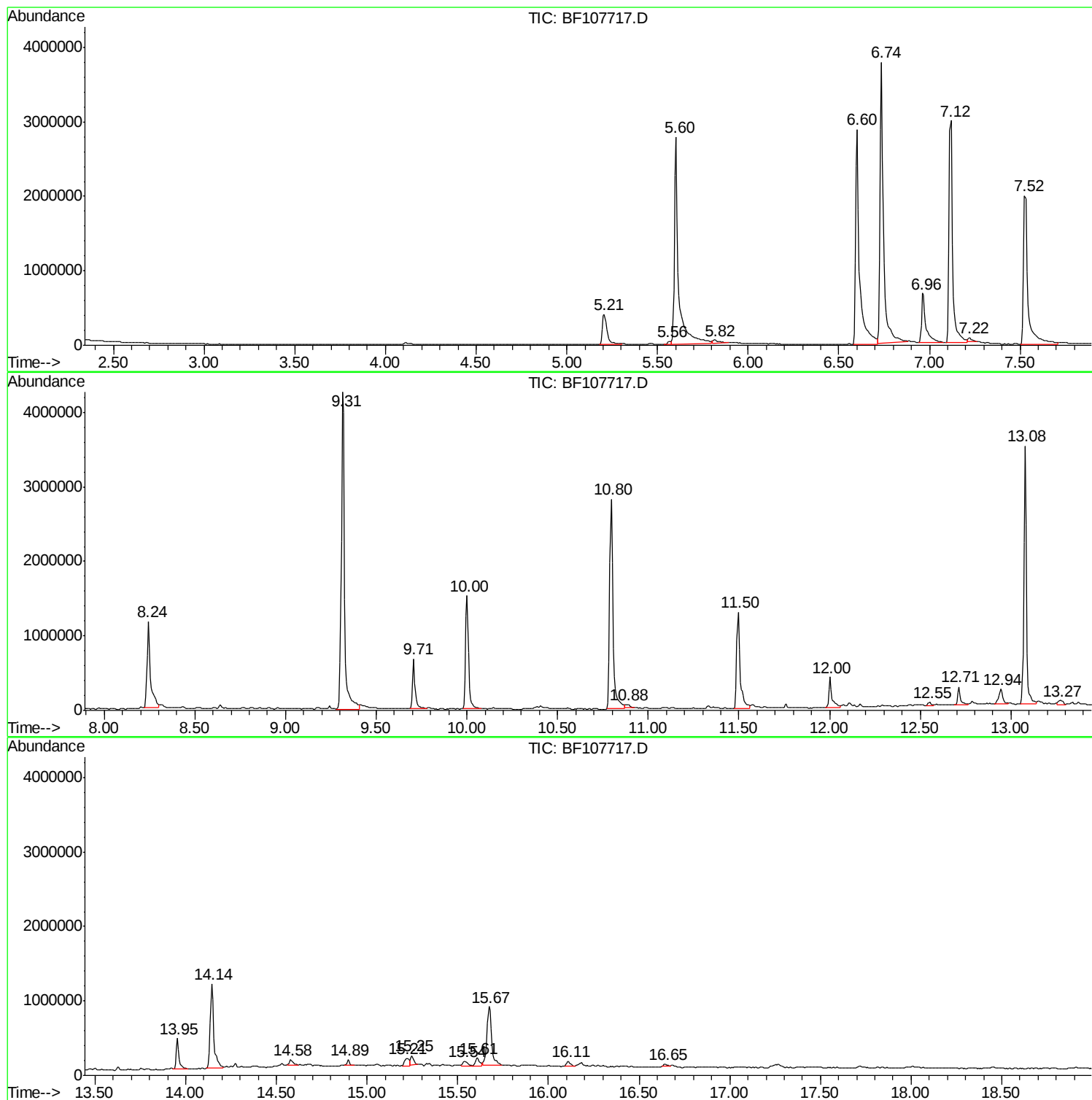
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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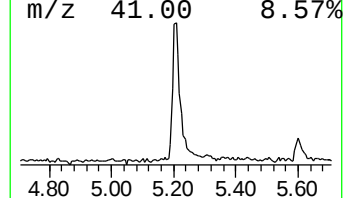
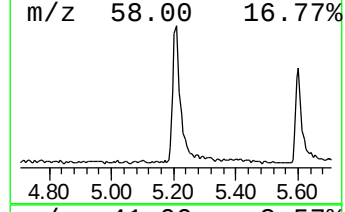
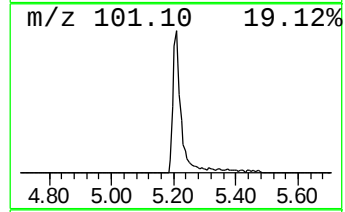
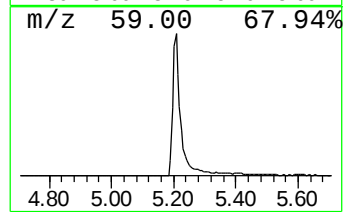
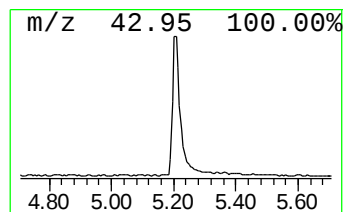
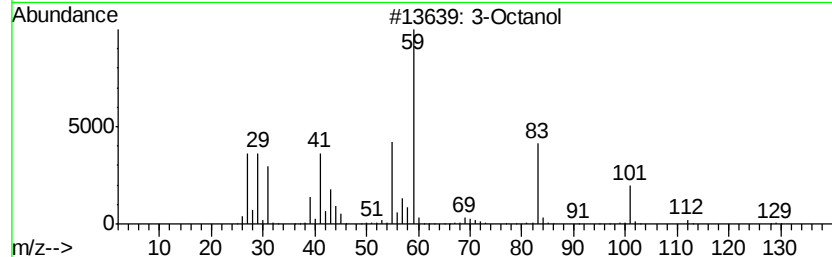
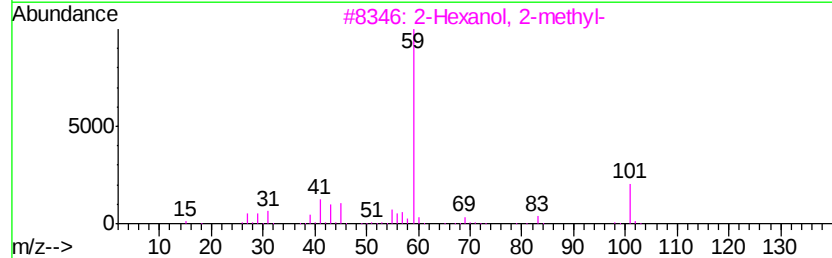
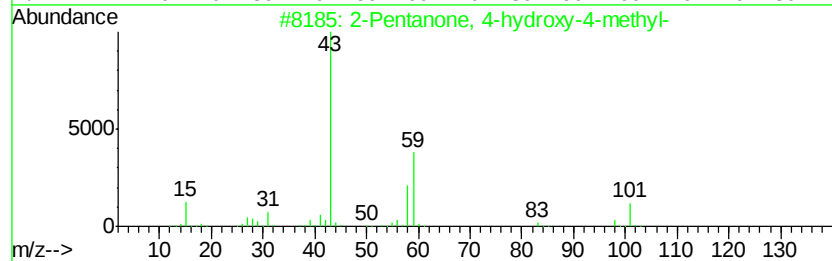
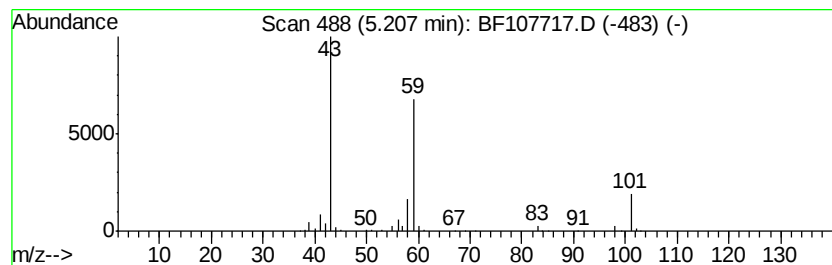
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	13.00 ng	711511	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	56
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3			3-Octanol	130	C8H18O	000589-98-0	33
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



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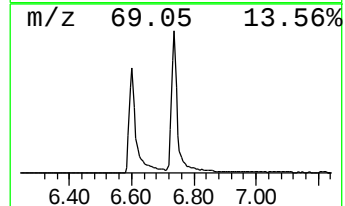
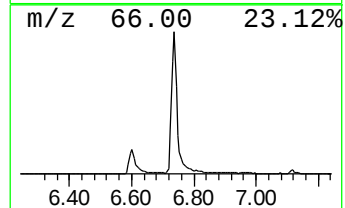
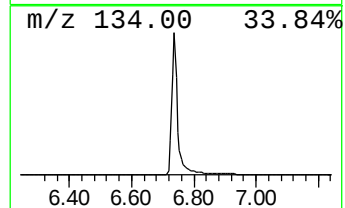
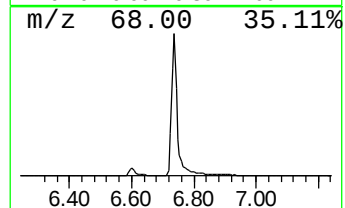
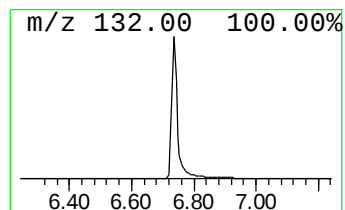
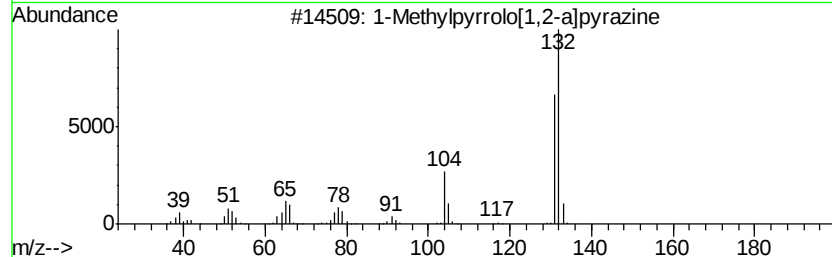
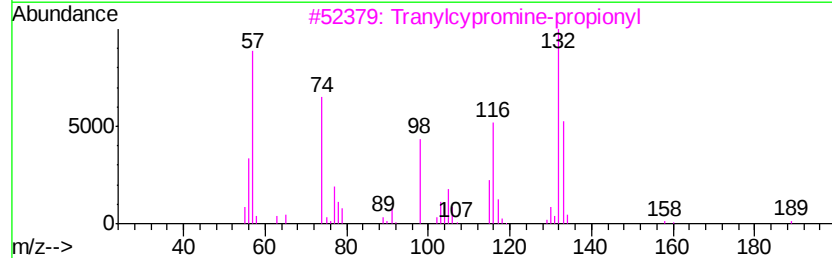
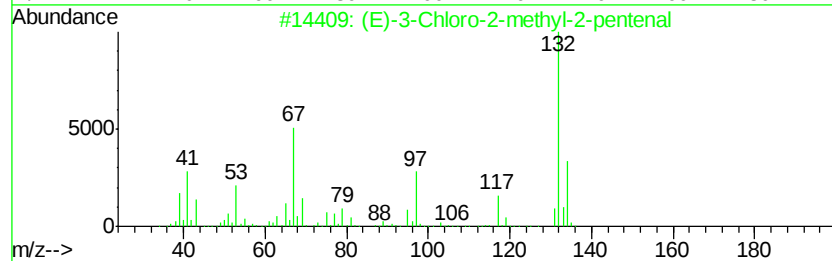
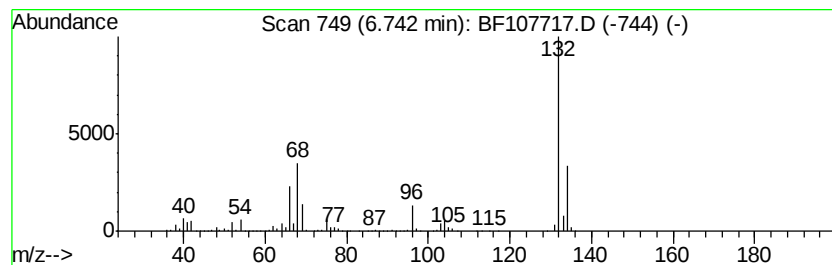
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Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	90.55 ng	4956720	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		5-Aminoindole	132	C8H8N2	005192-03-0	9



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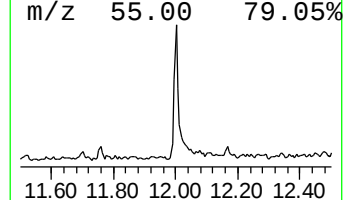
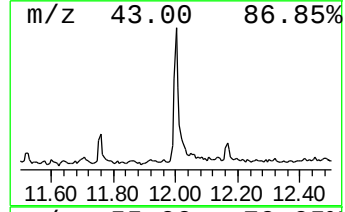
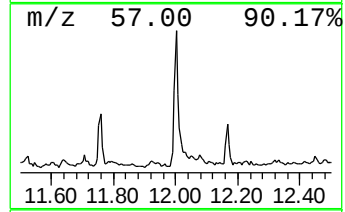
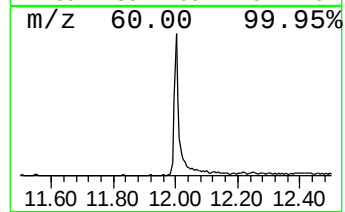
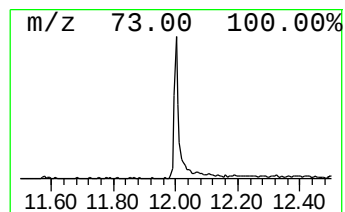
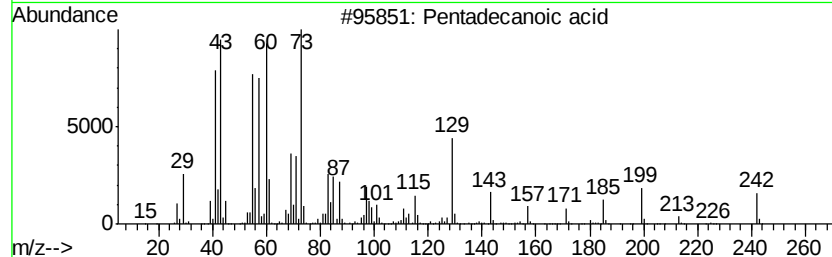
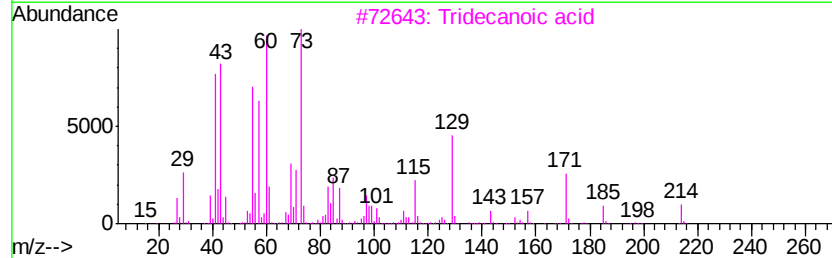
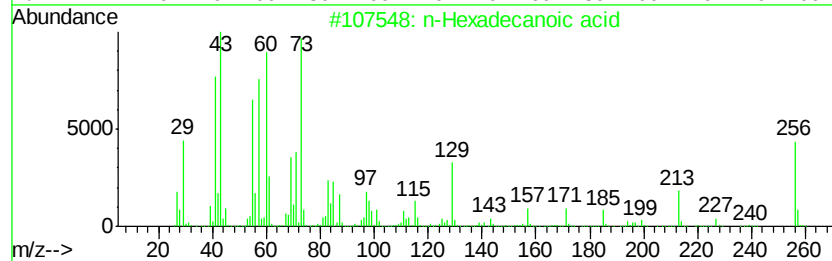
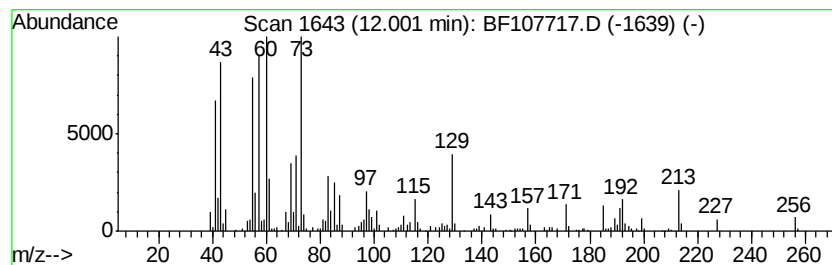
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	6.38 ng	518981	Phenanthrene-d10	11.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Tridecanoic acid	214	C13H26O2	000638-53-9	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5		n-Decanoic acid	172	C10H20O2	000334-48-5	70



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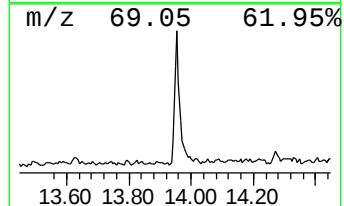
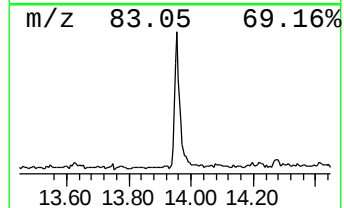
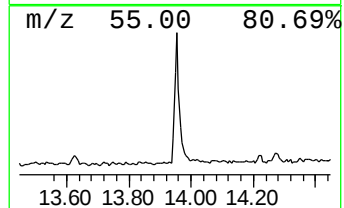
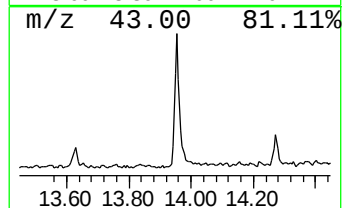
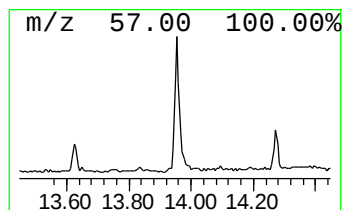
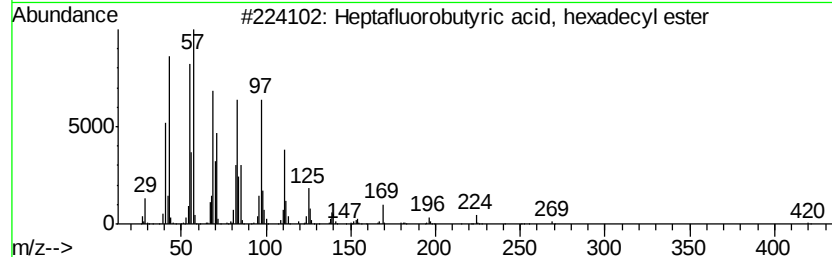
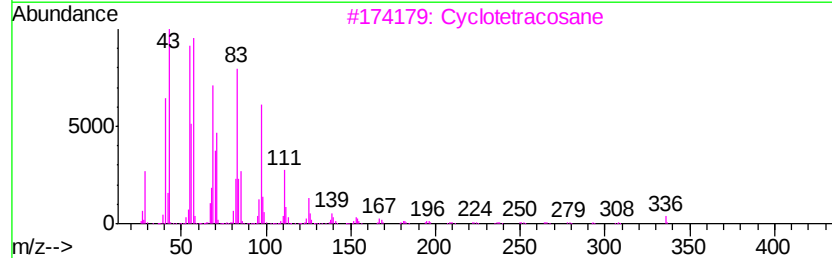
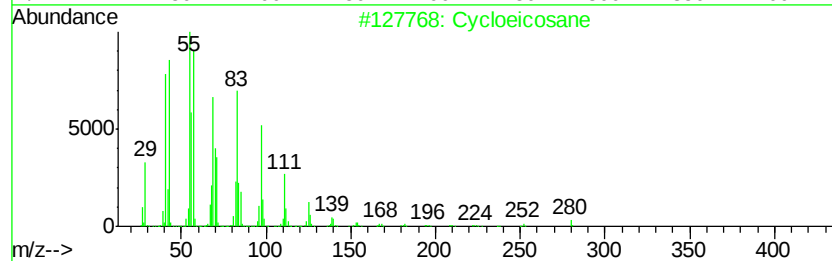
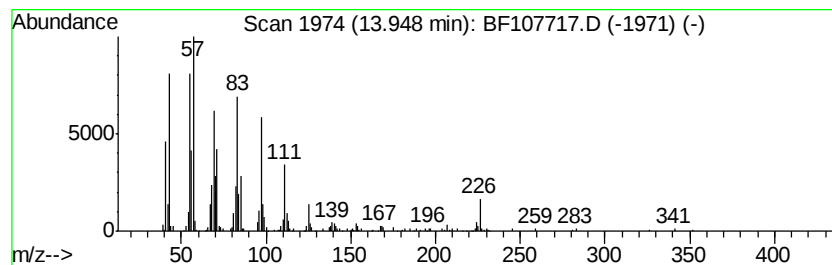
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Peak Number 5 Cycloeicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	6.40 ng	470765	Chrysene-d12	14.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cycloeicosane	280	C20H40	000296-56-0	97
2		Cyclotetracosane	336	C24H48	000297-03-0	95
3		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
4		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.21	13.0	ng	711511	1	6.97	1094840	20.0
unknown6.74	6.74	90.5	ng	4956720	1	6.97	1094840	20.0
n-Hexadecanoic acid	12.00	6.4	ng	518981	4	11.50	1626210	20.0
Cycloeicosane	13.95	6.4	ng	470765	5	14.14	1470960	20.0