

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082118\
 Data File : BF108330.D
 Acq On : 21 Aug 2018 11:17
 Operator : JU/SJ
 Sample : J4500-24
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ROCK

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-BF080818.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	3.231	147	152	159	rVB	67673	95254	1.30%	0.187%
2	5.278	495	500	512	rVB	677622	963101	13.15%	1.892%
3	5.654	559	564	567	rBV	4505996	4848535	66.19%	9.523%
4	6.637	725	731	734	rBV	4225776	4563291	62.30%	8.962%
5	6.784	750	756	759	rBV	5235942	5365406	73.25%	10.538%
6	7.007	790	794	797	rBV	1229539	1060526	14.48%	2.083%
7	7.166	816	821	824	rBV	4526693	4215046	57.55%	8.278%
8	7.572	883	890	893	rBV	3334127	3738247	51.04%	7.342%
9	8.289	1007	1012	1015	rBV	1297124	1327122	18.12%	2.606%
10	9.366	1188	1195	1198	rBV	5758107	6443540	87.97%	12.655%
11	10.048	1306	1311	1315	rBV2	1590197	1539871	21.02%	3.024%
12	10.848	1440	1447	1450	rBV	4230305	4475810	61.11%	8.791%
13	11.548	1560	1566	1569	rBV	1839269	1706096	23.29%	3.351%
14	12.930	1797	1801	1805	rBV	211924	170271	2.32%	0.334%
15	13.136	1829	1836	1839	rBV	6517898	7324639	100.00%	14.386%
16	13.636	1918	1921	1925	rBV	140672	112106	1.53%	0.220%
17	14.201	2012	2017	2020	rBV	1642530	1458370	19.91%	2.864%
18	15.324	2204	2208	2214	rVB	77000	95389	1.30%	0.187%
19	15.754	2274	2281	2291	rVB2	737416	1098315	14.99%	2.157%
20	16.212	2354	2359	2366	rVB2	99436	166793	2.28%	0.328%
21	16.771	2447	2454	2461	rBV	77245	148602	2.03%	0.292%

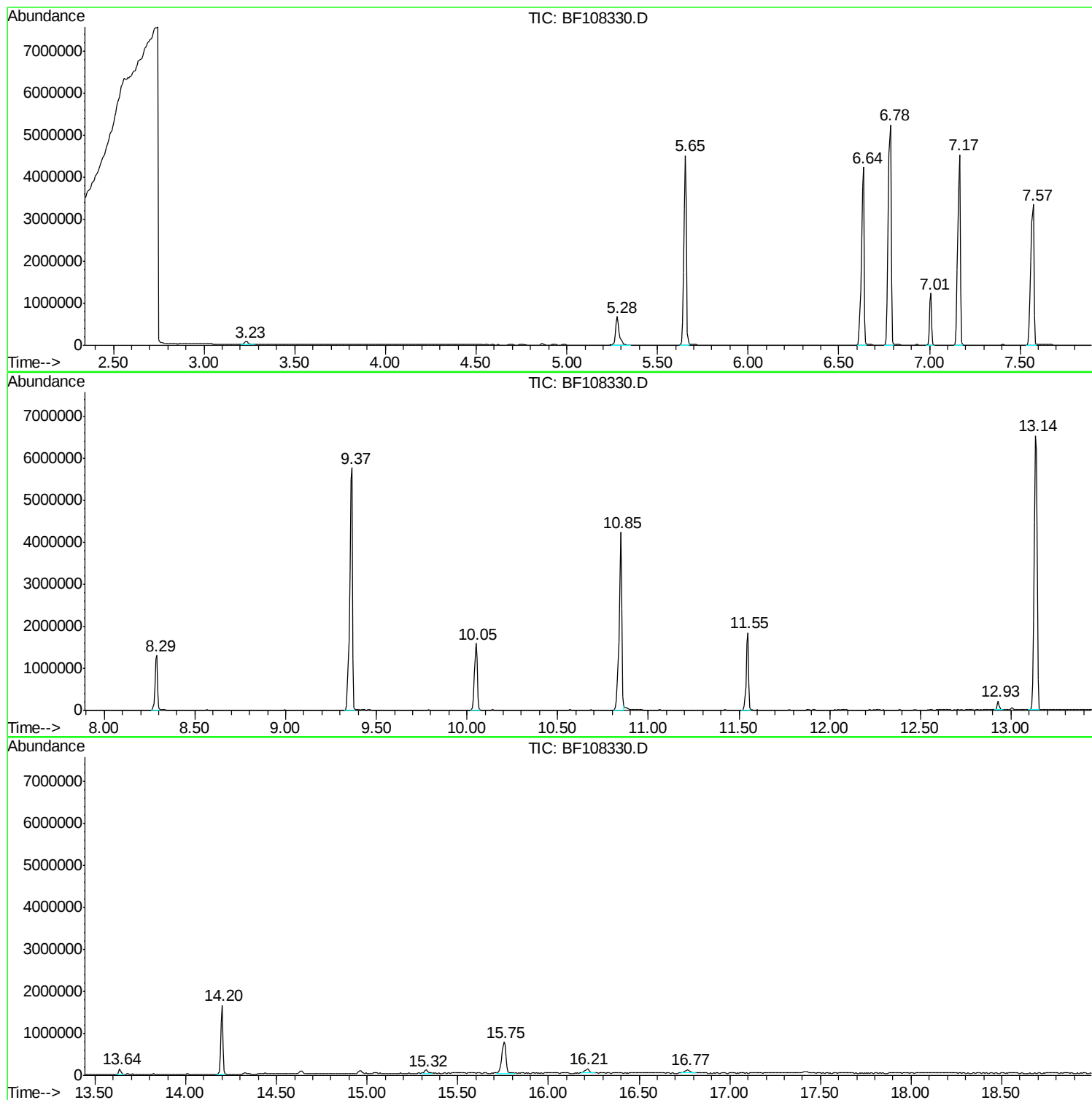
Sum of corrected areas: 50916330

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.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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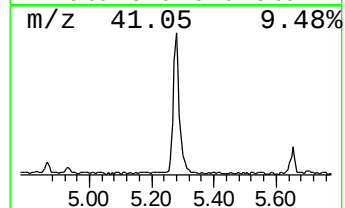
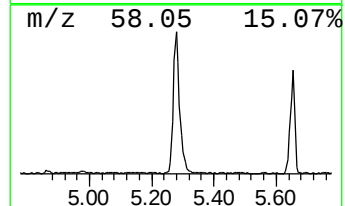
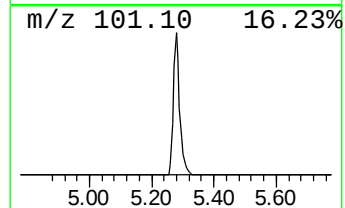
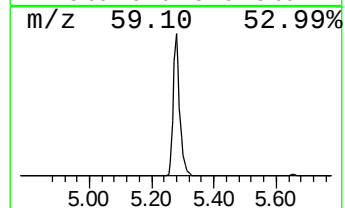
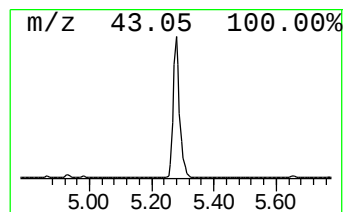
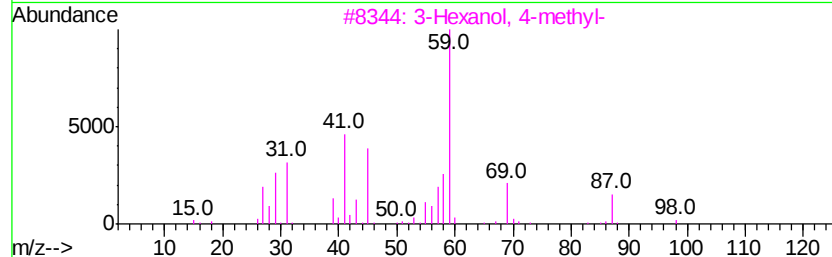
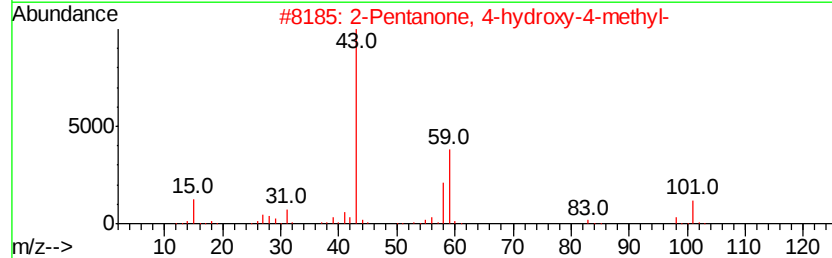
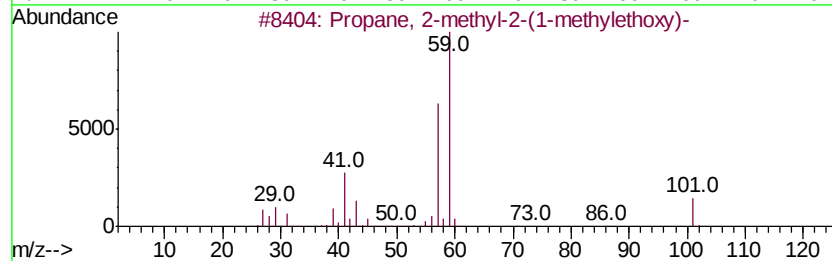
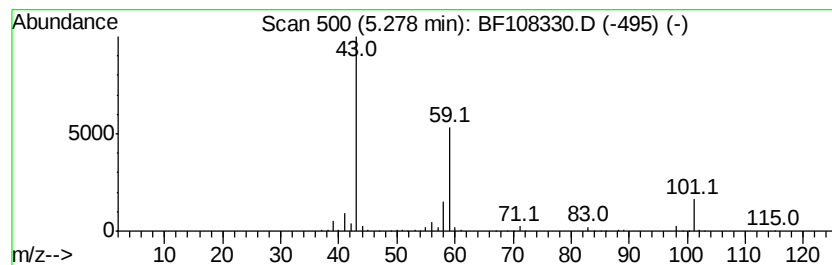
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.28	18.16 ng	963101	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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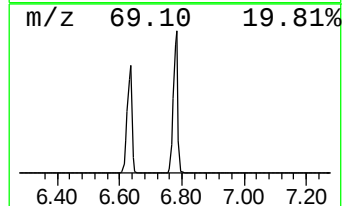
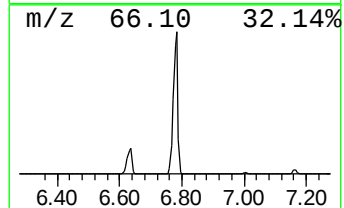
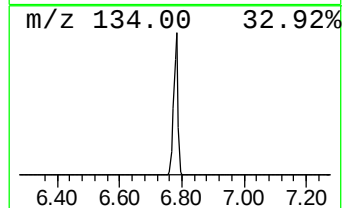
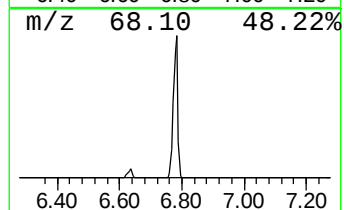
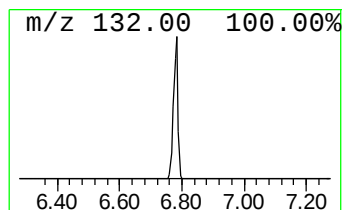
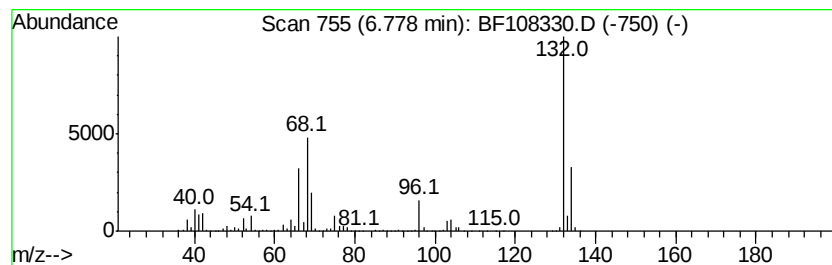
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.78 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	101.18 ng	5365410	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcvpromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Xenon	132	Xe	007440-63-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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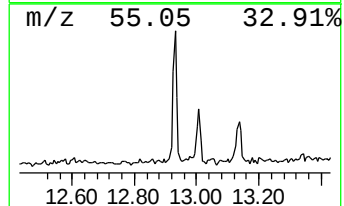
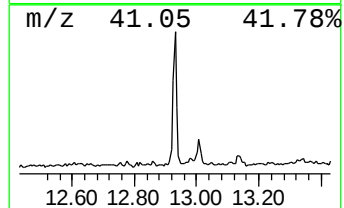
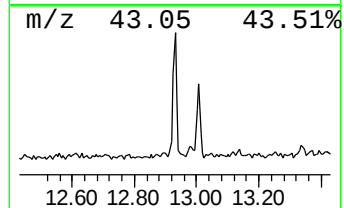
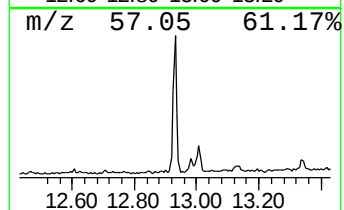
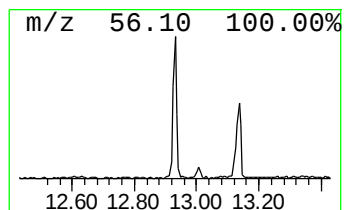
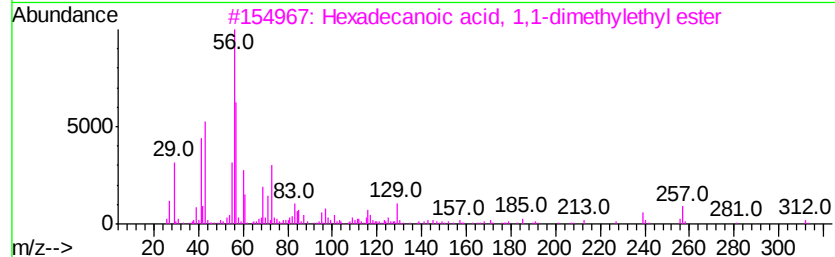
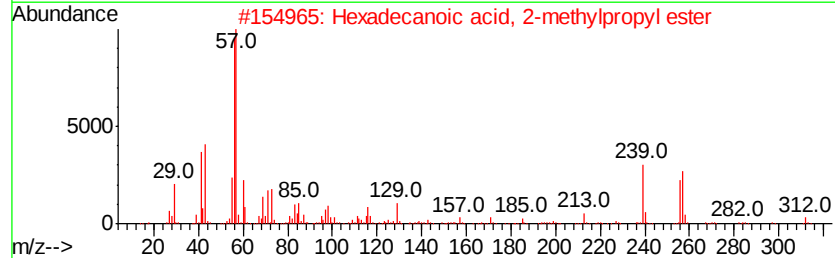
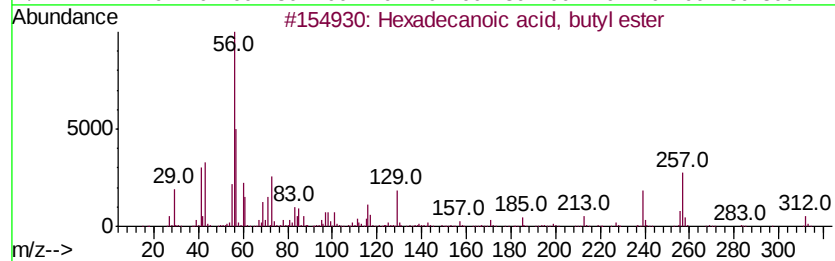
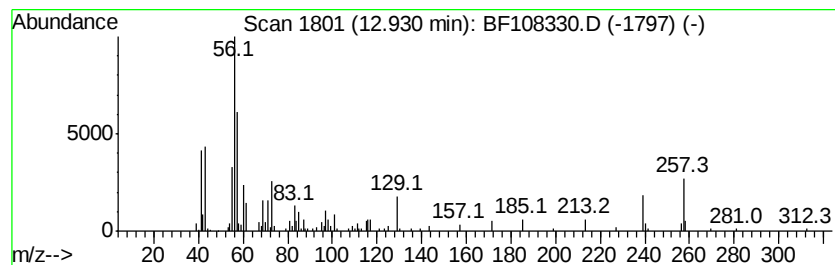
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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.93	2.34 ng	170271	Chrysene-d12	14.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	46
3		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	35
4		Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	35
5		Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32



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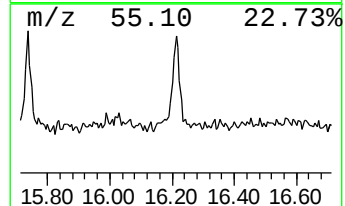
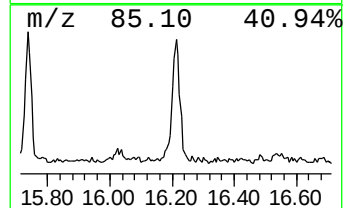
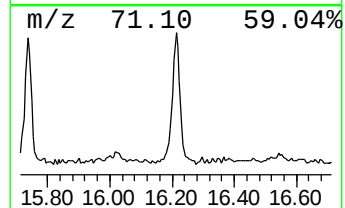
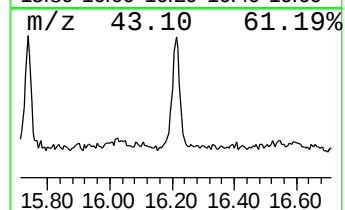
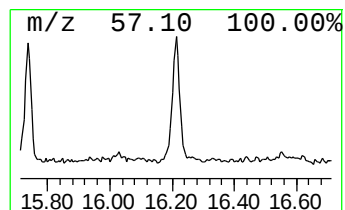
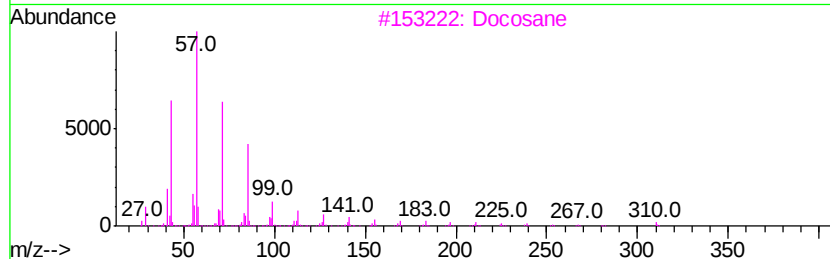
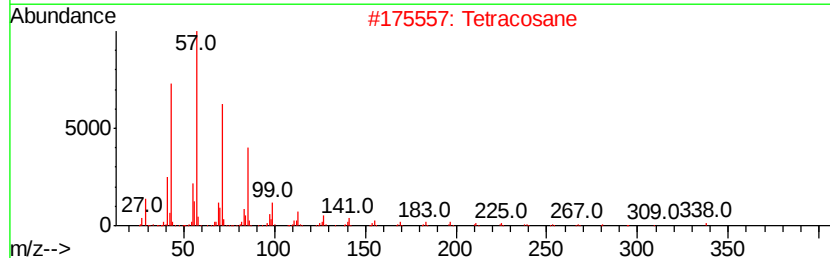
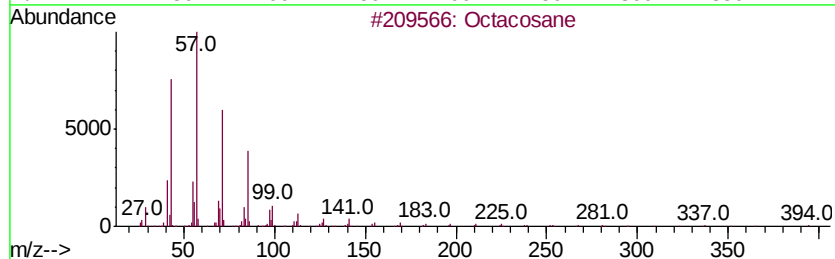
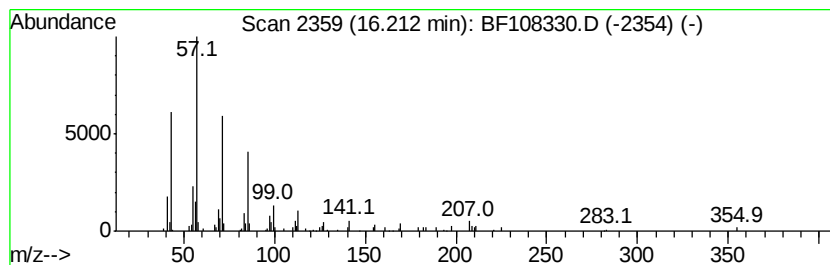
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 Peak Number 5 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.21	3.04 ng	166793	Perylene-d12	15.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	90
2	Tetracosane		338	C24H50	000646-31-1	90
3	Docosane		310	C22H46	000629-97-0	90
4	Pentacosane		352	C25H52	000629-99-2	87
5	Heptacosane		380	C27H56	000593-49-7	87



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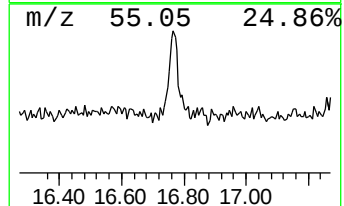
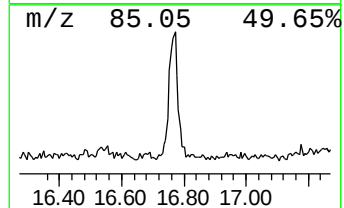
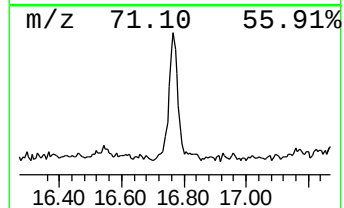
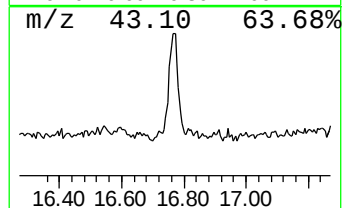
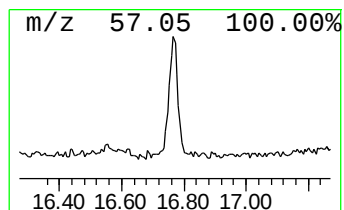
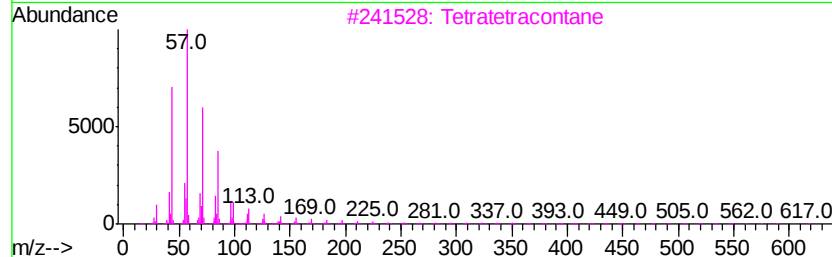
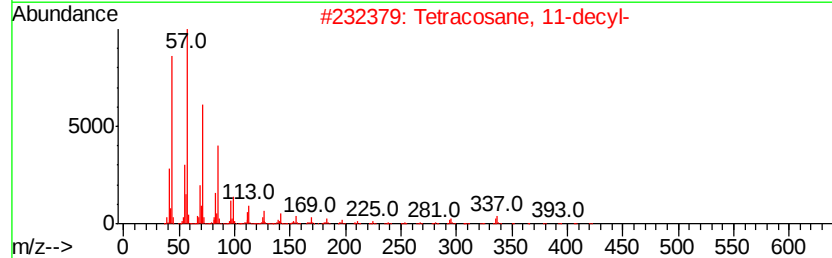
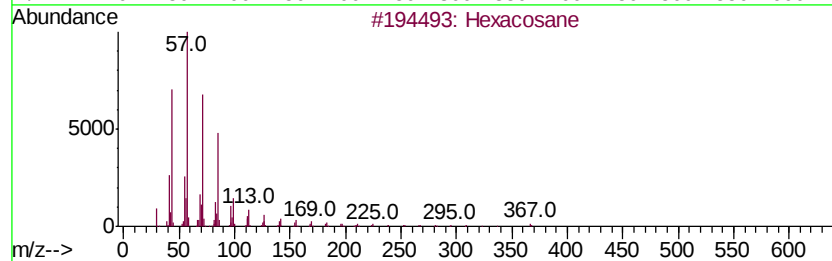
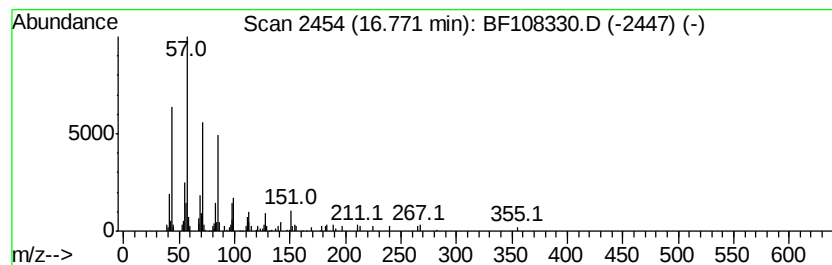
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Peak Number 6 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.77	2.71 ng	148602	Perylene-d12	15.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	90
2	Tetracosane, 11-decyl-		479	C34H70	055429-84-0	87
3	Tetratetracontane		619	C44H90	007098-22-8	87
4	Tetracosane		338	C24H50	000646-31-1	86
5	Heneicosane		296	C21H44	000629-94-7	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.28	18.2	ng	963101	1	7.01	1060530	20.0
unknown6.78	6.78	101.2	ng	5365410	1	7.01	1060530	20.0
Hexadecanoic acid...	12.93	2.3	ng	170271	5	14.20	1458370	20.0
Octacosane	16.21	3.0	ng	166793	6	15.75	1098320	20.0
Hexacosane	16.77	2.7	ng	148602	6	15.75	1098320	20.0