

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052916\
 Data File : BF087575.D
 Acq On : 31 May 2016 5:37
 Operator : UM/SJ
 Sample : H3316-06
 Misc :
 ALS Vial : 93 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-07-COMP

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-BF052316.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	4.719	271	274	294	rBV	96976	350012	9.61%	1.300%
2	5.382	330	332	352	rBV	1398018	2930989	80.45%	10.886%
3	7.039	474	477	483	rBV	1975202	2834671	77.81%	10.529%
4	7.130	483	485	510	rVV	2094895	3643175	100.00%	13.532%
5	7.473	513	515	526	rVV	475091	778556	21.37%	2.892%
6	7.702	532	535	551	rVB	1777756	2376772	65.24%	8.828%
7	8.388	593	595	626	rBV	1236794	2025991	55.61%	7.525%
8	9.508	690	693	710	rBV	489782	984384	27.02%	3.656%
9	11.279	845	848	864	rBV	2440919	3288052	90.25%	12.213%
10	11.988	908	910	918	rBV	61067	117340	3.22%	0.436%
11	12.331	938	940	951	rBV	631631	977252	26.82%	3.630%
12	13.154	1007	1012	1015	rBV2	31225	40364	1.11%	0.150%
13	13.634	1051	1054	1075	rBV2	698733	1571181	43.13%	5.836%
14	13.931	1077	1080	1085	rVB	35401	54043	1.48%	0.201%
15	14.743	1149	1151	1166	rVV	471881	801771	22.01%	2.978%
16	16.926	1340	1342	1345	rBV	148020	155921	4.28%	0.579%
17	17.086	1354	1356	1366	rBV	1959844	2358671	64.74%	8.761%
18	17.851	1421	1423	1426	rBV	92743	104726	2.87%	0.389%
19	18.331	1463	1465	1472	rBV4	23745	89603	2.46%	0.333%
20	18.469	1474	1477	1485	rBV	355206	720907	19.79%	2.678%
21	19.554	1570	1572	1574	rBV	32419	44411	1.22%	0.165%
22	19.840	1595	1597	1599	rBV	30765	43339	1.19%	0.161%
23	20.160	1622	1625	1633	rBV2	215111	631370	17.33%	2.345%

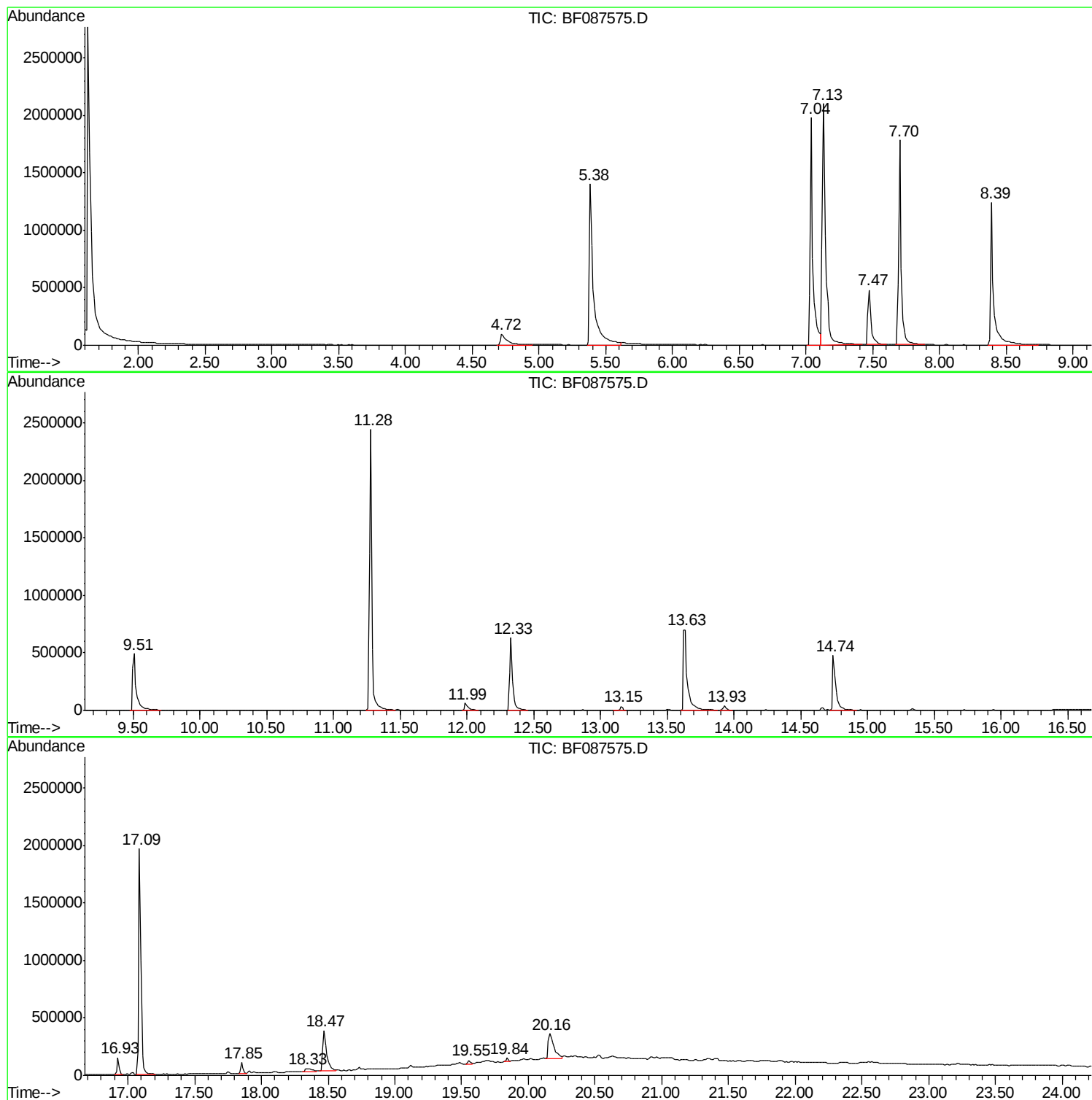
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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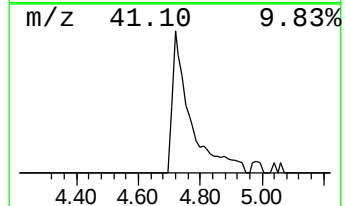
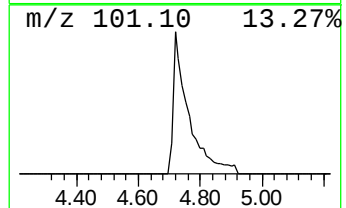
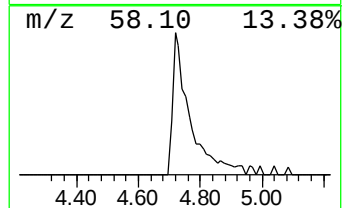
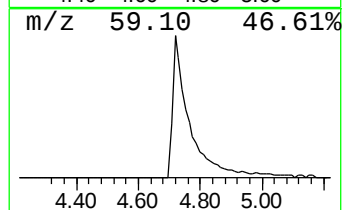
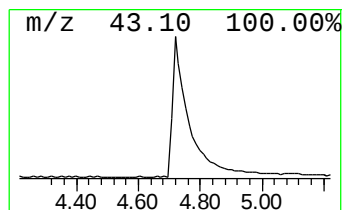
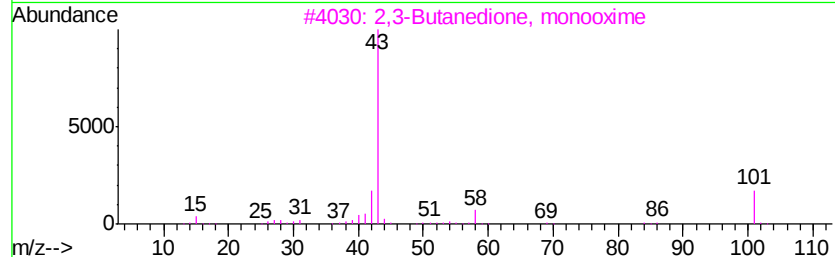
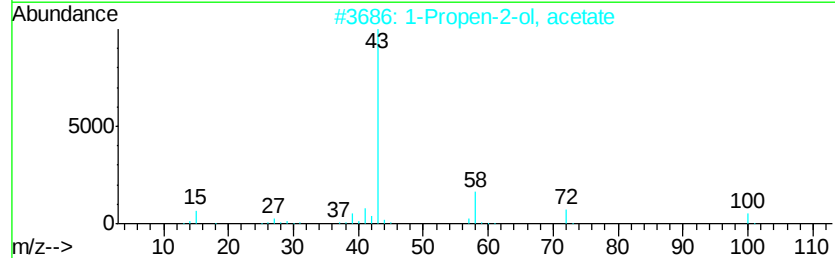
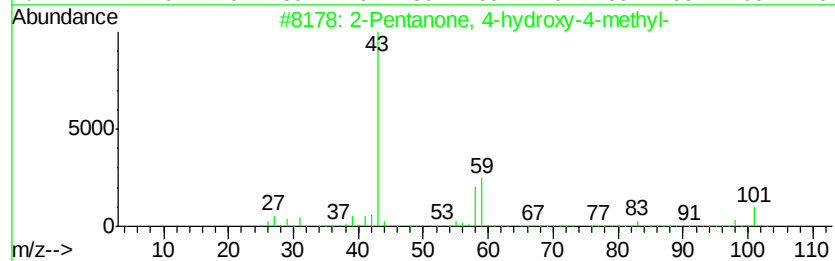
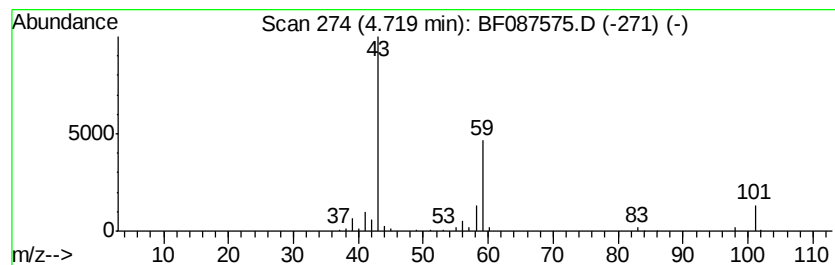
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.72	8.99 ng	350012	1,4-Dichlorobenzene-d4	7.47

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10	
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	
4	Butane	58	C4H10	000106-97-8	9	
5	Diacetamide	101	C4H7NO2	000625-77-4	9	



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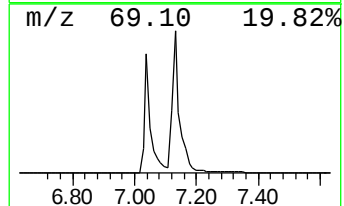
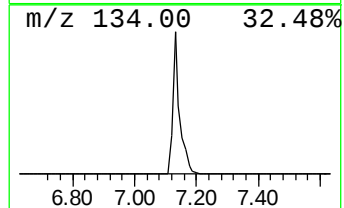
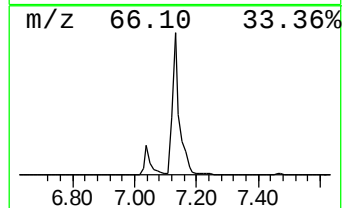
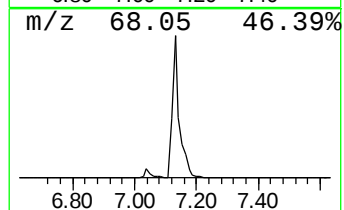
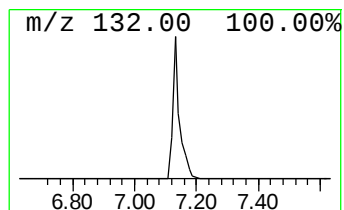
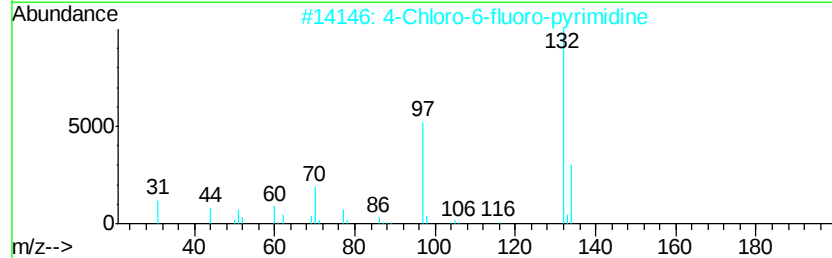
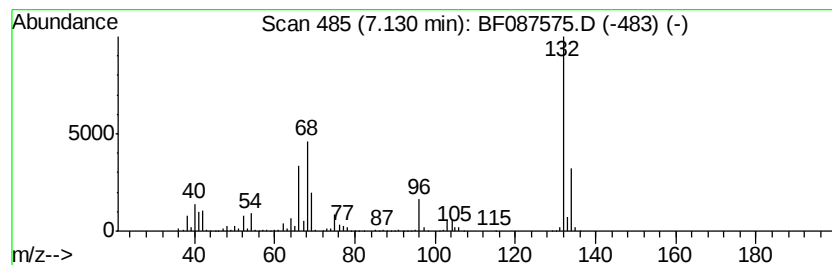
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF052316.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.13 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.13	93.59 ng	3643180	1,4-Dichlorobenzene-d4	7.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	22
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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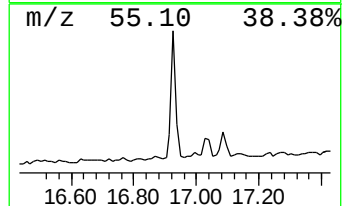
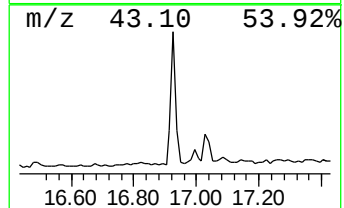
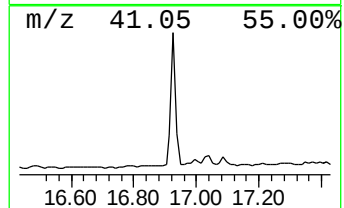
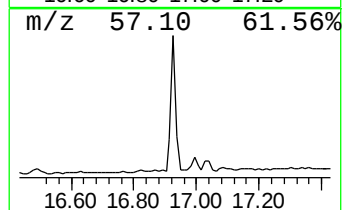
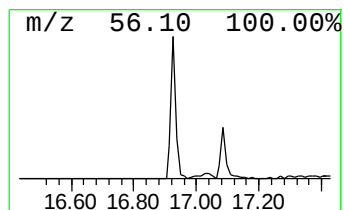
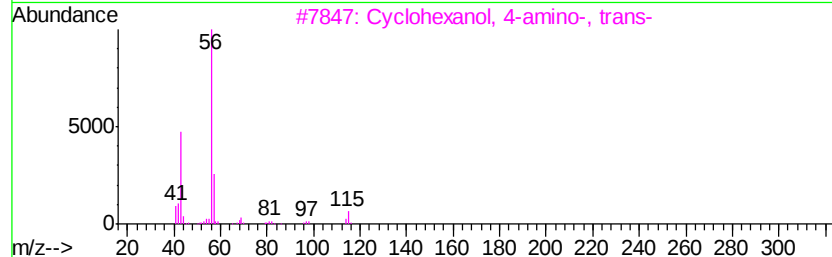
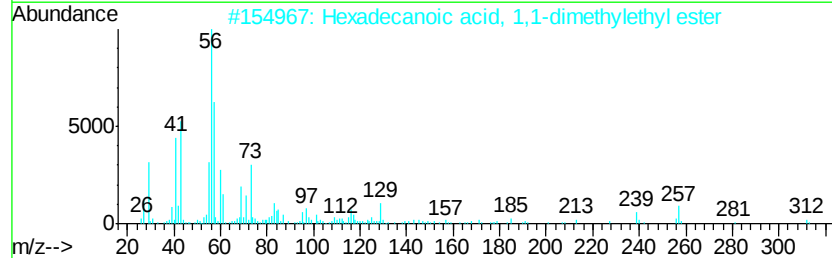
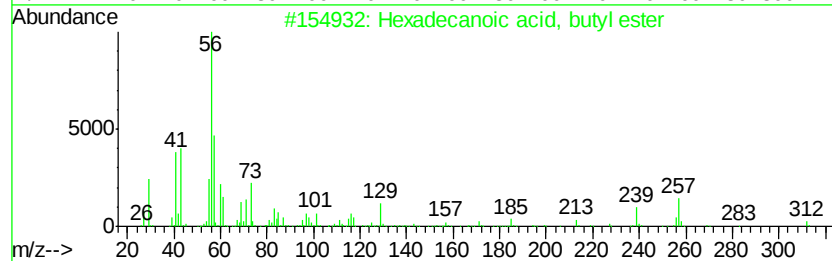
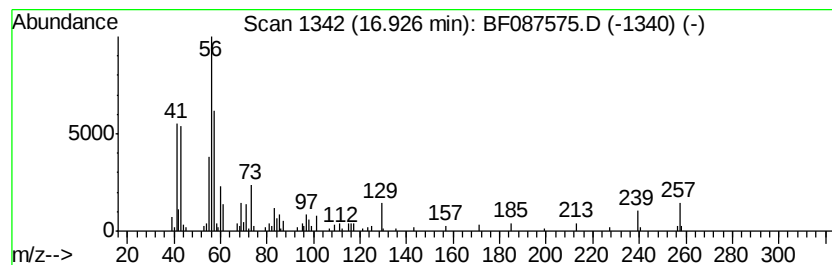
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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.93	4.33 ng	155921	Chrysene-d12	18.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	49
3		Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	38
4		Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35
5		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35



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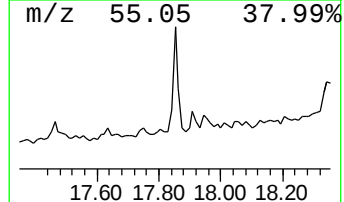
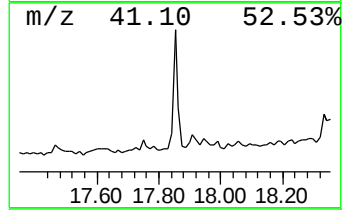
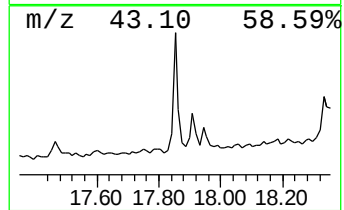
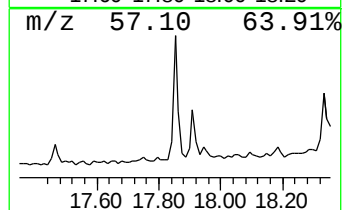
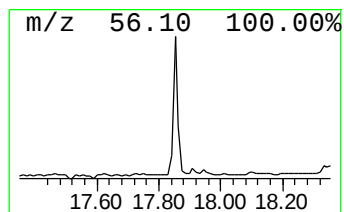
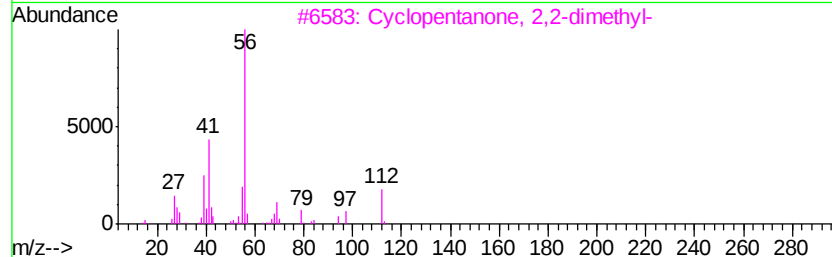
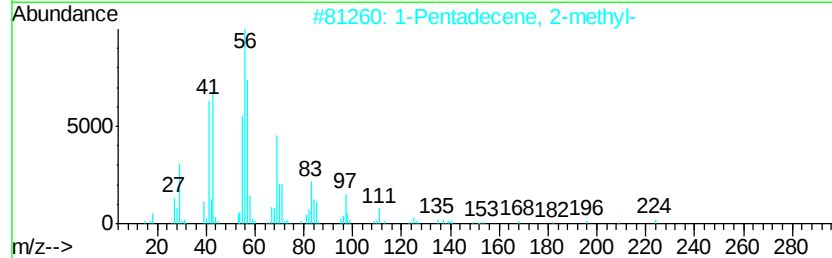
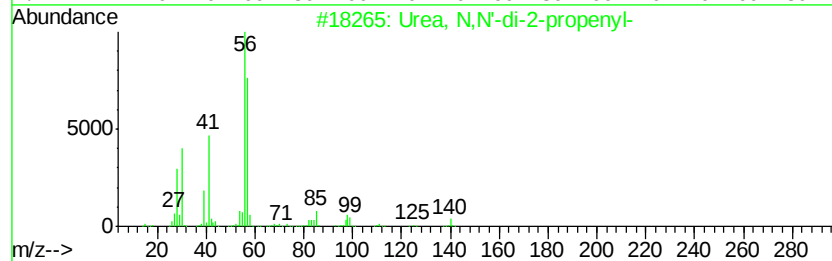
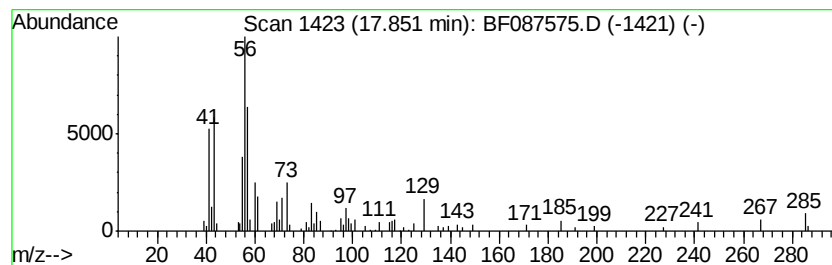
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Peak Number 5 unknown17.85 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.85	2.91 ng	104726	Chrysene-d12	18.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	43
2	1-Pentadecene, 2-methyl-	224	C16H32	029833-69-0	43
3	Cyclopentanone, 2,2-dimethyl-	112	C7H12O	004541-32-6	38
4	4,7,7-Trimethyl-3,9-dioxatricycl...	182	C10H14O3	1000187-22-5	37
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35



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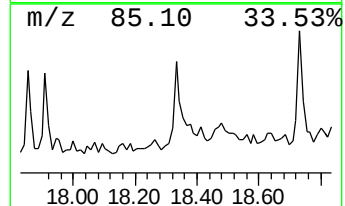
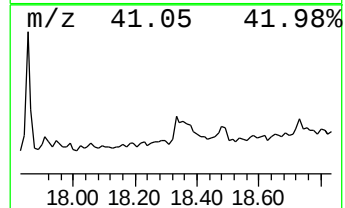
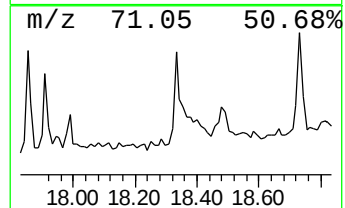
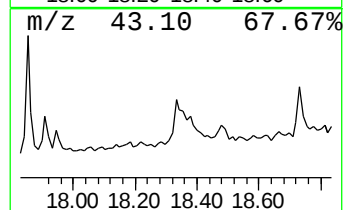
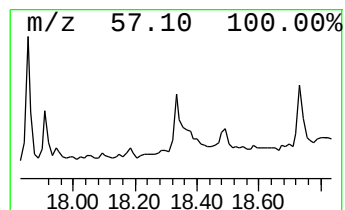
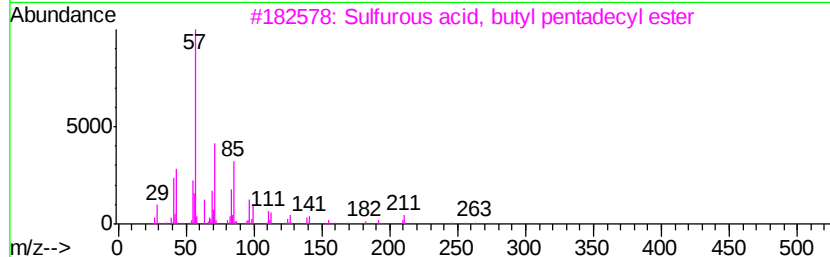
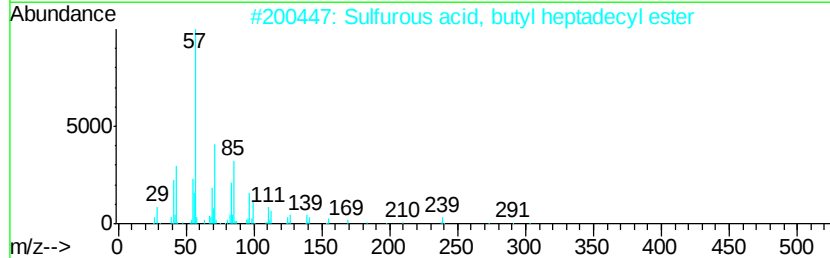
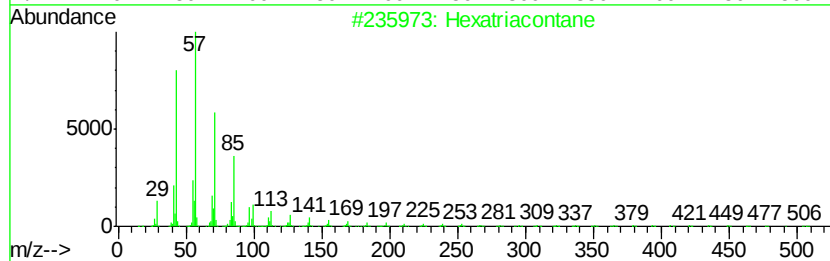
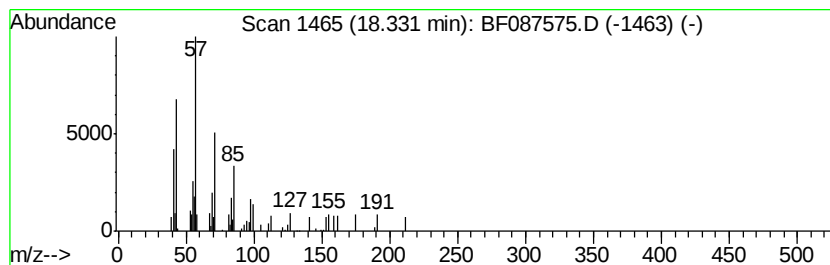
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Peak Number 6 Hexatriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.33	2.49 ng	89603	Chrysene-d12	18.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexatriacontane	507	C36H74	000630-06-8	80
2		Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	80
3		Sulfurous acid, butyl pentadecyl...	348	C19H40O3S	1000309-18-2	80
4		Heptacosane	380	C27H56	000593-49-7	72
5		Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.72	9.0	ng	350012	1	7.47	778556	20.0
unknown7.13	7.13	93.6	ng	3643180	1	7.47	778556	20.0
Hexadecanoic acid...	16.93	4.3	ng	155921	5	18.47	720907	20.0
unknown17.85	17.85	2.9	ng	104726	5	18.47	720907	20.0
Hexatriacontane	18.33	2.5	ng	89603	5	18.47	720907	20.0