

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122916\
 Data File : BF092025.D
 Acq On : 29 Dec 2016 15:45
 Operator : UM/SJ
 Sample : H6281-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-6

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:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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	4.830	238	240	249	rVB	684663	854749	10.16%	1.461%
2	5.299	278	281	293	rBV	3372503	3351581	39.86%	5.728%
3	6.350	371	373	381	rBV	2545451	2330104	27.71%	3.982%
4	6.464	381	383	386	rBV	6184187	5963696	70.92%	10.192%
5	6.693	400	403	405	rBV	1490792	1672543	19.89%	2.858%
6	6.853	414	417	419	rBV	4505914	6119788	72.78%	10.458%
7	7.265	449	453	455	rBV	5056771	5693160	67.70%	9.729%
8	7.973	513	515	518	rBV	2250070	2254997	26.82%	3.854%
9	9.059	607	610	612	rBV	7756359	8408839	100.00%	14.370%
10	9.459	643	645	647	rBV	212749	253441	3.01%	0.433%
11	9.733	666	669	670	rBV	1933574	2661448	31.65%	4.548%
12	10.156	704	706	710	rBV5	32954	85824	1.02%	0.147%
13	10.248	710	714	717	rBV	148437	227115	2.70%	0.388%
14	10.522	735	738	740	rBV	4443590	4971916	59.13%	8.497%
15	10.648	747	749	753	rVB2	69872	153644	1.83%	0.263%
16	11.082	786	787	792	rBV3	50033	114212	1.36%	0.195%
17	11.208	796	798	804	rVB	2170365	2078165	24.71%	3.551%
18	11.345	808	810	812	rBV2	58207	110083	1.31%	0.188%
19	11.471	818	821	823	rBV	167865	318228	3.78%	0.544%
20	11.665	835	838	839	rBV3	82705	156592	1.86%	0.268%
21	11.756	844	846	850	rVB3	339650	457558	5.44%	0.782%
22	12.545	912	915	921	rBV	253998	337296	4.01%	0.576%
23	12.808	934	938	940	rBV	4746518	6934451	82.47%	11.851%
24	13.699	1014	1016	1021	rVB3	99047	156454	1.86%	0.267%
25	13.837	1026	1028	1031	rBV	1475453	1570706	18.68%	2.684%
26	15.220	1146	1149	1152	rBV	872842	1279263	15.21%	2.186%

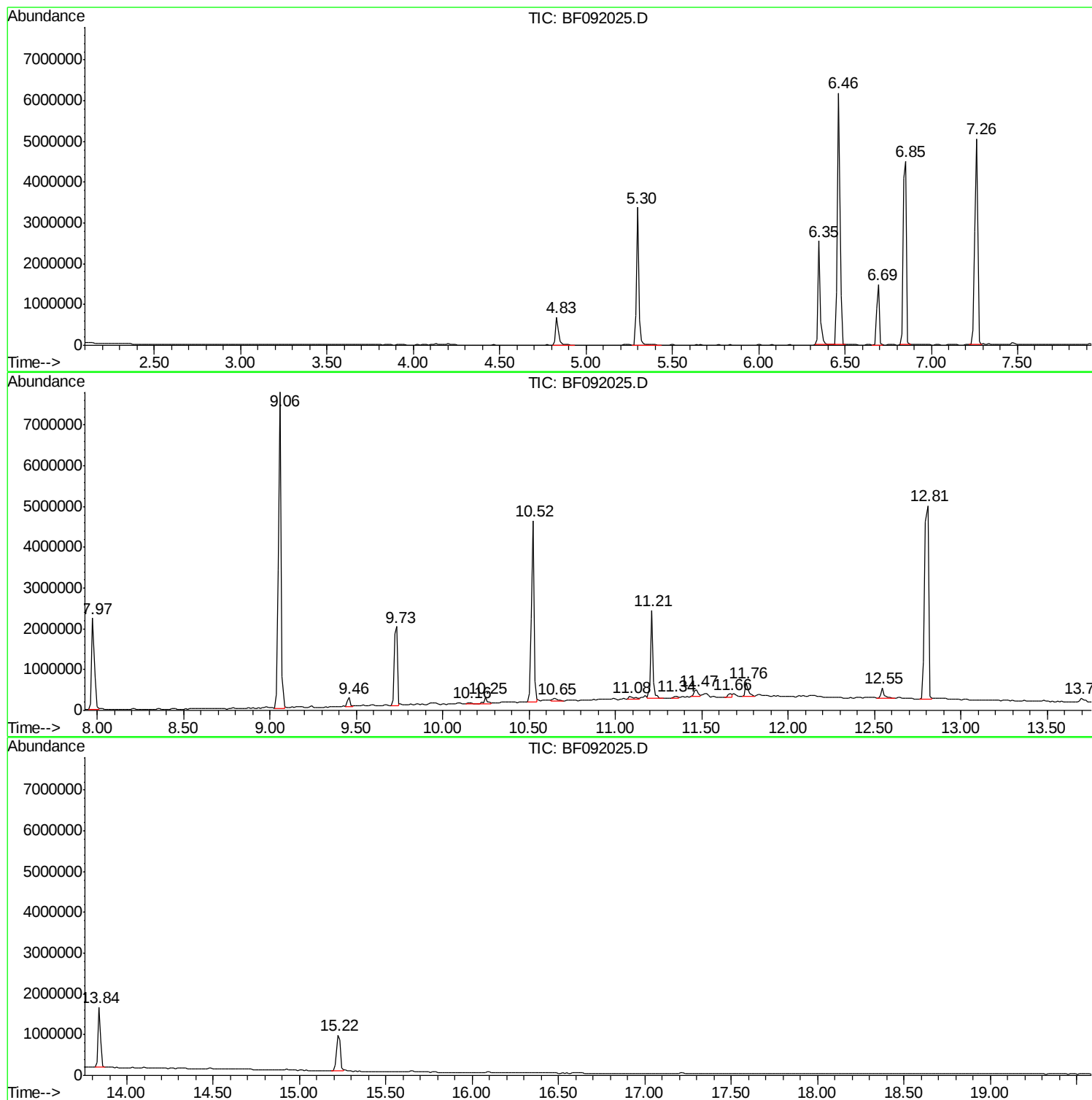
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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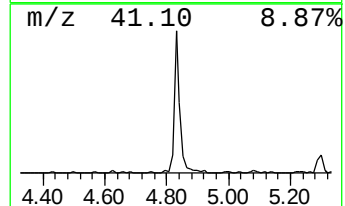
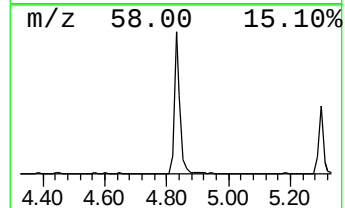
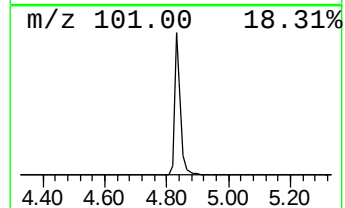
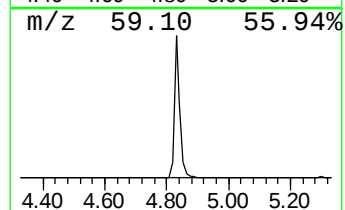
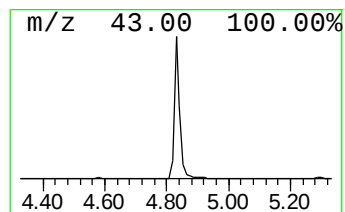
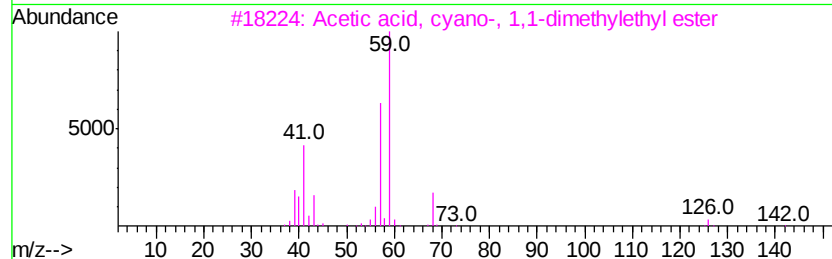
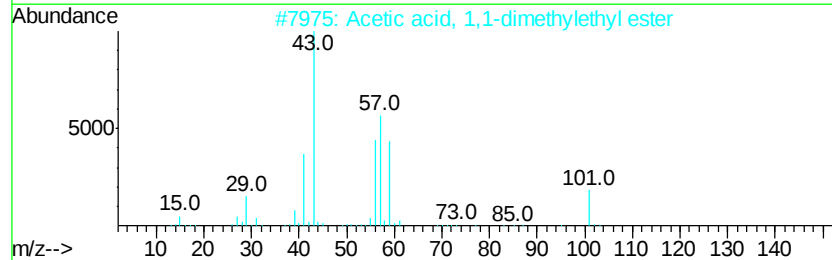
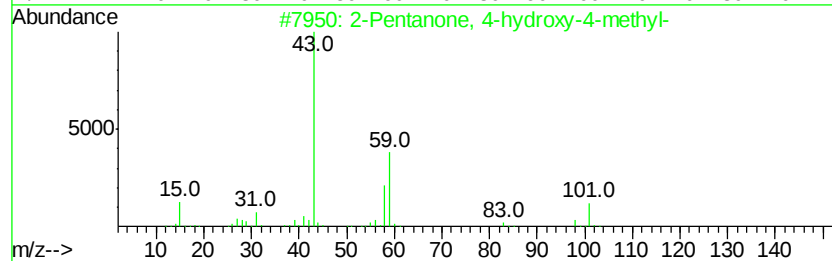
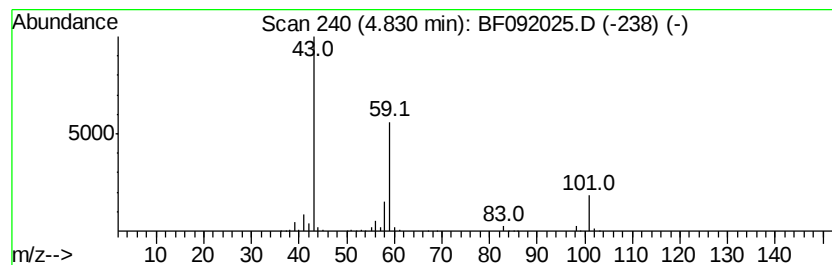
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.	
4.83	10.22 ng	854749	1,4-Dichlorobenzene-d4	6.69	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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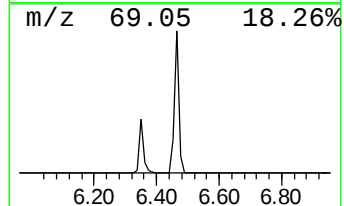
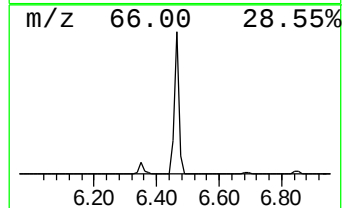
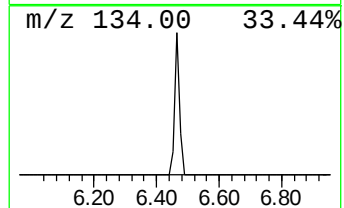
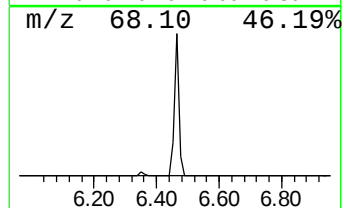
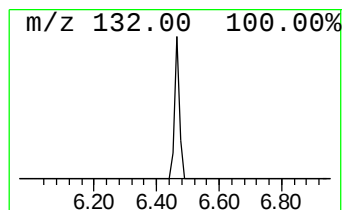
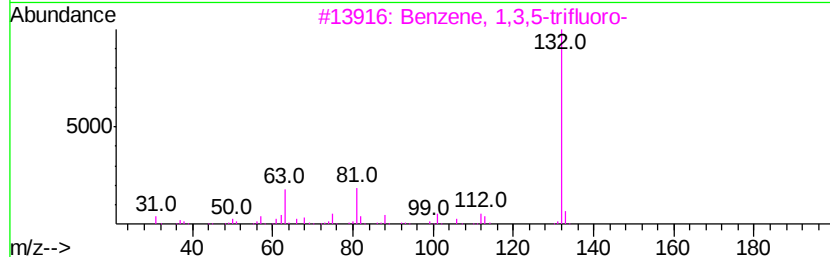
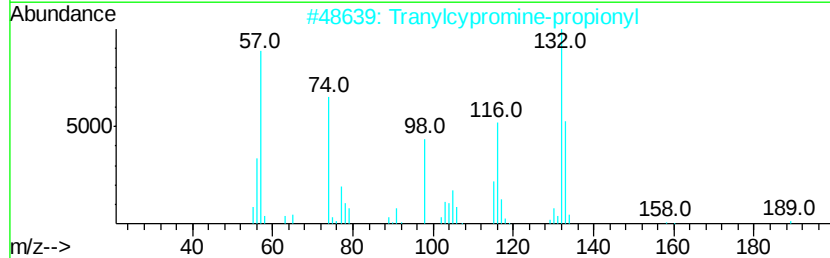
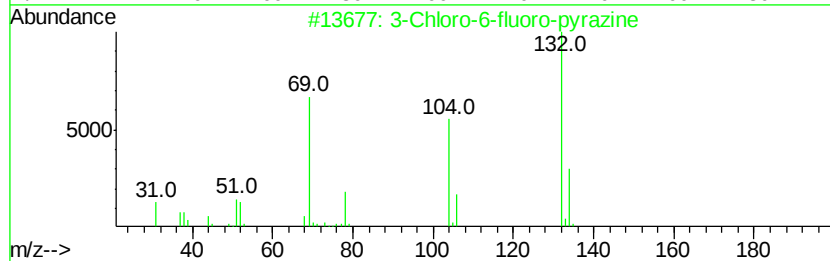
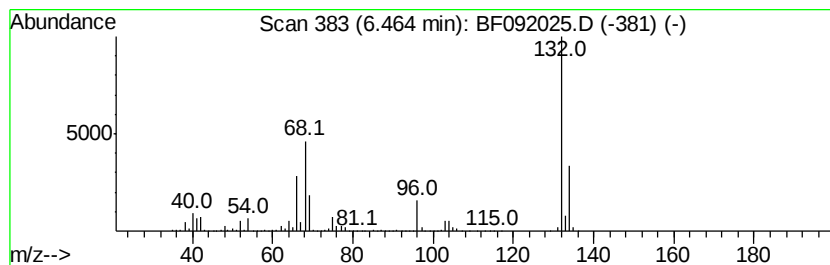
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.46 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	71.31 ng	5963700	1,4-Dichlorobenzene-d4	6.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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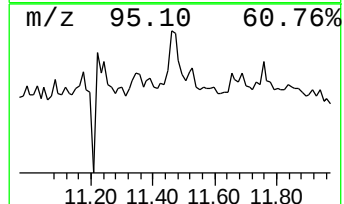
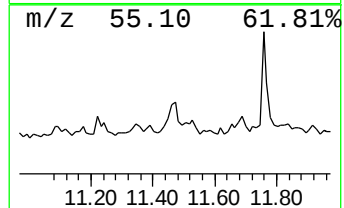
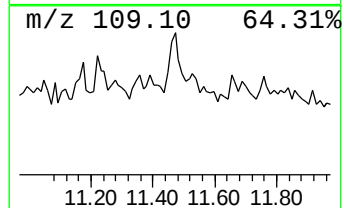
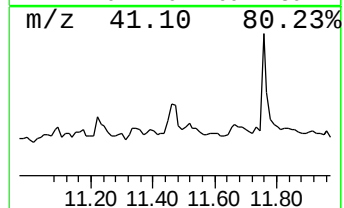
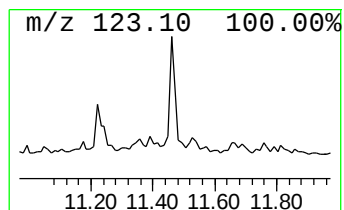
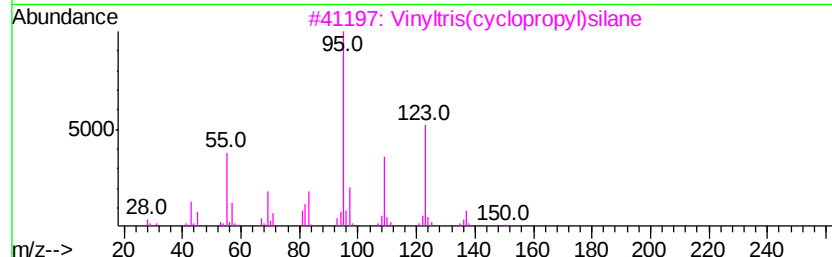
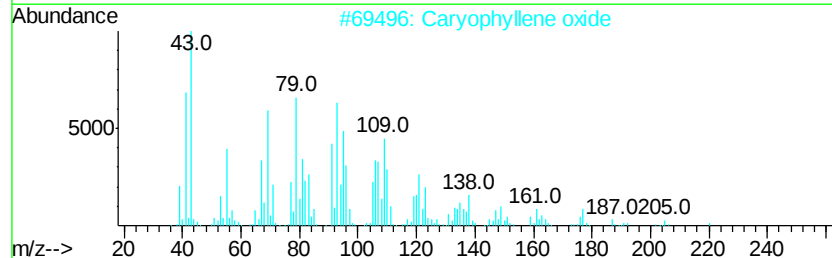
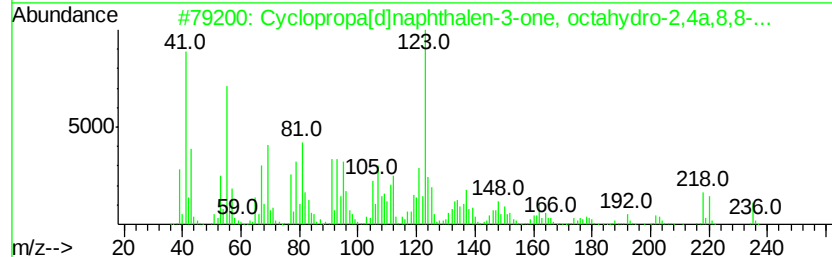
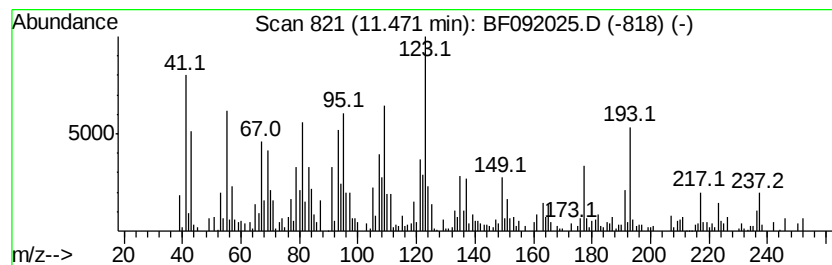
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Peak Number 4 unknown11.47 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.47	3.06 ng	318228	Phenanthrene-d10	11.21	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cvclopropa[d]lnaphthalen-3-one, o...	235	C15H25NO	024703-24-0	38
2	Carvophyllene oxide	220	C15H24O	001139-30-6	30
3	Vinyltris(cvclopropyl)silane	178	C11H18Si	1000109-97-3	27
4	Benzamide, 4-fluoro-N-(5H-tetraz...	207	C8H6FN5O	1000262-68-4	22
5	2,2-Dimethylocta-3,4-dienal	152	C10H16O	000590-71-6	22



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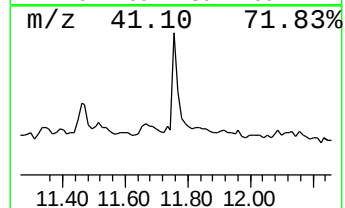
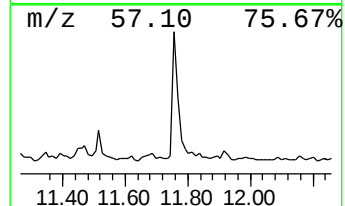
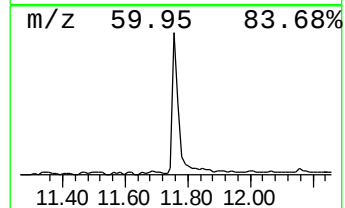
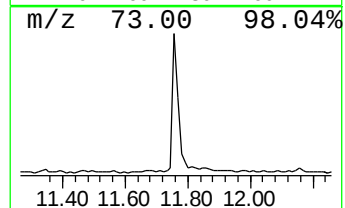
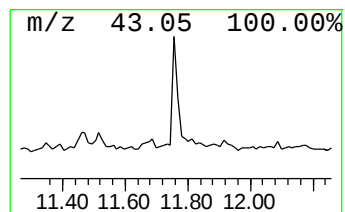
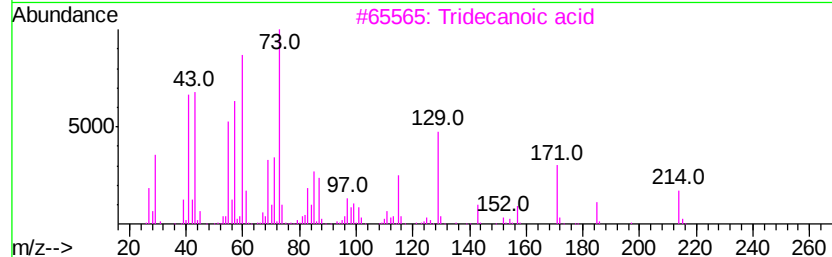
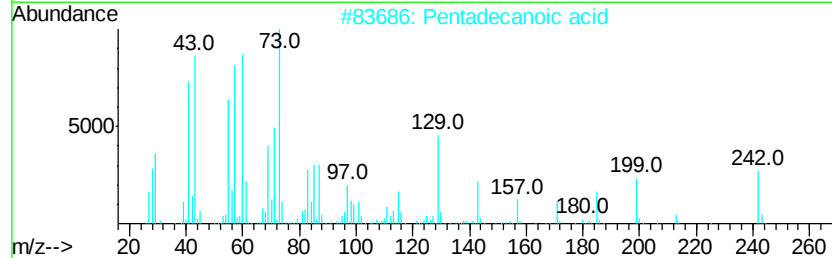
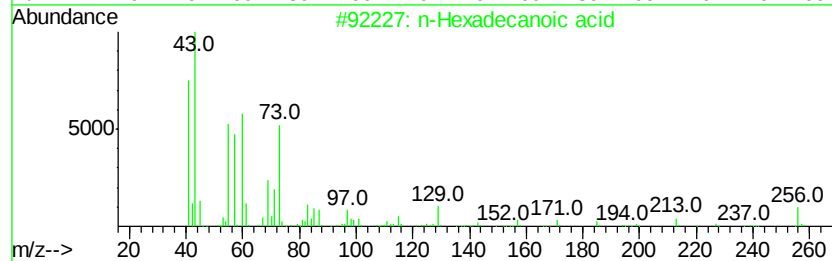
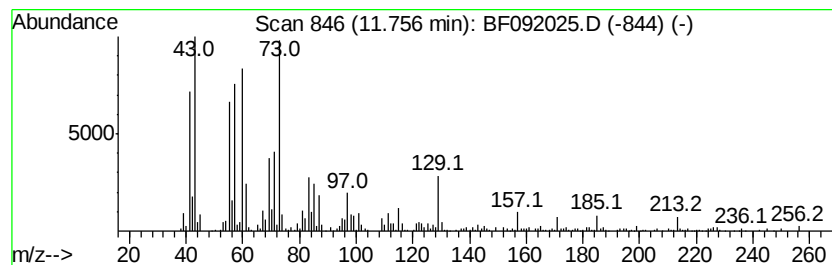
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.76	4.40 ng	457558	Phenanthrene-d10	11.21	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	Hexadecane	226	C16H34	000544-76-3	53
5	Methyl 2,6-anhydro-.alpha.-d-alt...	176	C7H12O5	1000130-02-0	22



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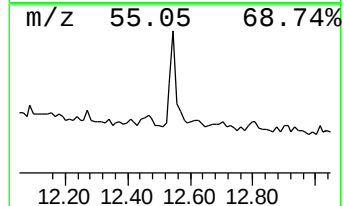
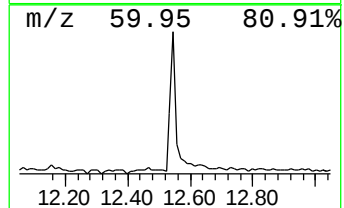
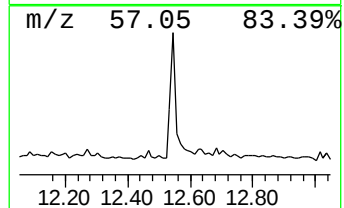
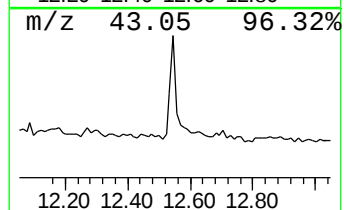
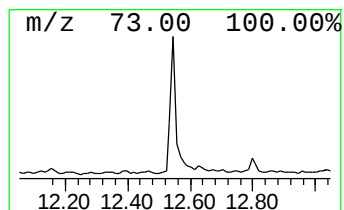
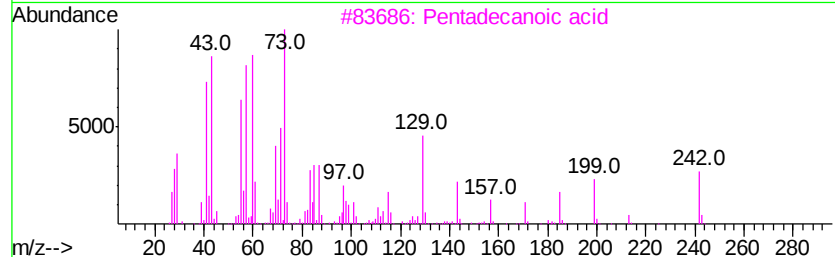
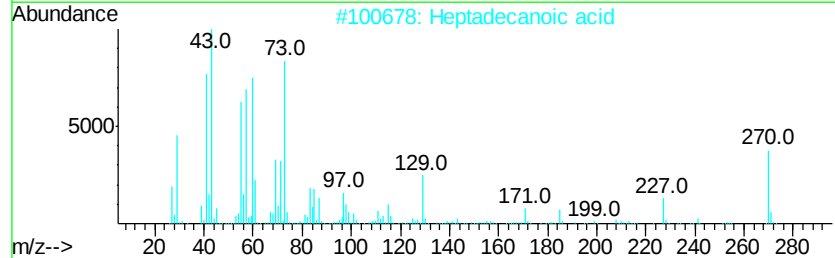
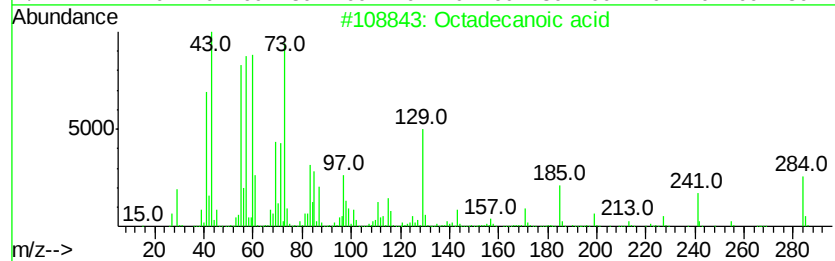
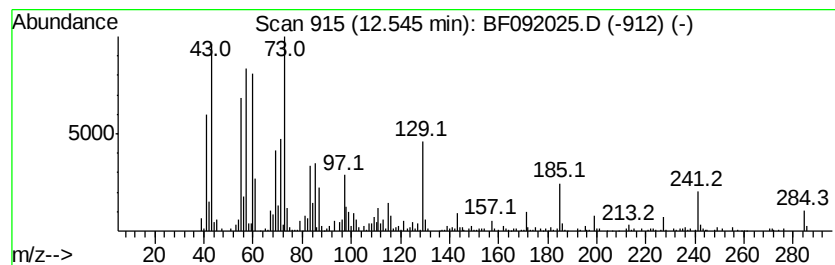
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Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.55	4.29 ng	337296	Chrysene-d12		13.84	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Heptadecanoic acid	270	C17H34O2	000506-12-7	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5		Undecanoic acid	186	C11H22O2	000112-37-8	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.83	10.2	ng	854749	1	6.69	1672540	20.0
unknown6.46	6.46	71.3	ng	5963700	1	6.69	1672540	20.0
unknown11.47	11.47	3.1	ng	318228	4	11.21	2078170	20.0
n-Hexadecanoic acid	11.76	4.4	ng	457558	4	11.21	2078170	20.0
Octadecanoic acid	12.55	4.3	ng	337296	5	13.84	1570710	20.0