

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081716\
 Data File : BF089777.D
 Acq On : 17 Aug 2016 21:39
 Operator : UM/SJ
 Sample : H4490-04
 Misc :
 ALS Vial : 48 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 670-UNDERCLIFF-2

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-BF081616.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	1.667	6	7	16	rVB	1846396	3344516	15.03%	2.150%
2	1.793	16	18	26	rBV	10680549	22255064	100.00%	14.306%
3	4.844	282	285	292	rVB	2737031	3950091	17.75%	2.539%
4	5.279	320	323	326	rBV	9958852	11258599	50.59%	7.237%
5	5.690	358	359	362	rVB	192660	223779	1.01%	0.144%
6	6.330	412	415	418	rBV	9309152	11243894	50.52%	7.228%
7	6.467	424	427	429	rBV	9595471	13328640	59.89%	8.568%
8	6.696	445	447	449	rBV	4174327	3413432	15.34%	2.194%
9	6.856	458	461	463	rBV	11091580	10705540	48.10%	6.882%
10	7.267	493	497	499	rBV	5731673	8365165	37.59%	5.377%
11	7.987	557	560	562	rBV	3201441	4347784	19.54%	2.795%
12	9.062	651	654	657	rBV	11864801	14483770	65.08%	9.311%
13	9.462	686	689	691	rBV	3150388	2692929	12.10%	1.731%
14	9.736	710	713	715	rBV	4942704	5077183	22.81%	3.264%
15	10.513	778	781	784	rBV2	6743795	8502644	38.21%	5.466%
16	10.662	792	794	798	rBV	323148	440037	1.98%	0.283%
17	11.108	828	833	834	rBV2	210376	234622	1.05%	0.151%
18	11.211	839	842	844	rBV	5860044	5255175	23.61%	3.378%
19	11.725	885	887	888	rBV	220450	232739	1.05%	0.150%
20	11.759	888	890	901	rVB2	760047	1054474	4.74%	0.678%
21	12.799	978	981	984	rBV	11849017	13432282	60.36%	8.635%
22	13.737	1060	1063	1069	rBV	365304	847158	3.81%	0.545%
23	13.839	1069	1072	1074	rBV	5255211	5069255	22.78%	3.259%
24	15.245	1192	1195	1198	rBV	3604070	4102793	18.44%	2.637%
25	17.908	1423	1428	1437	rBV	674640	1700104	7.64%	1.093%

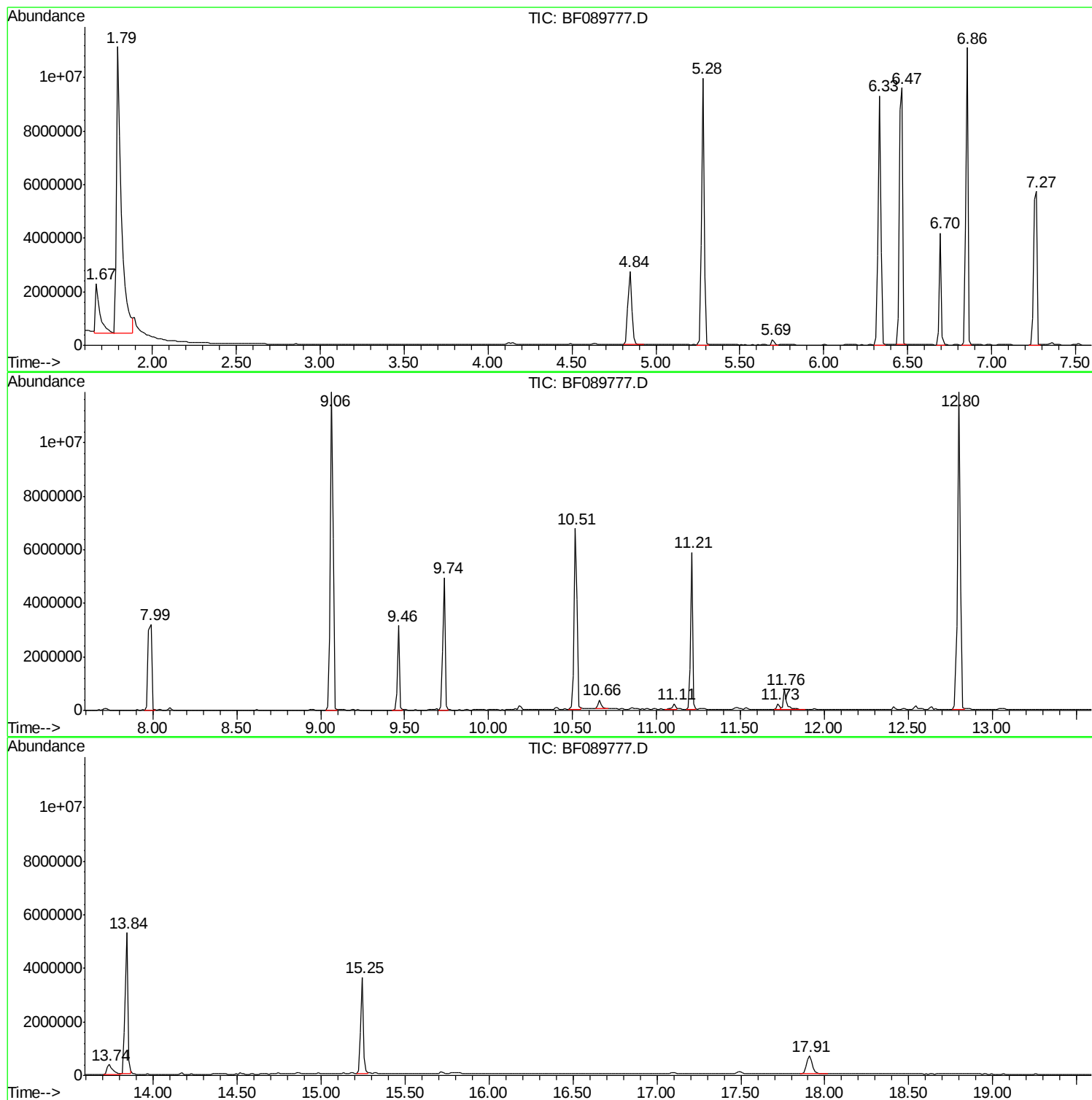
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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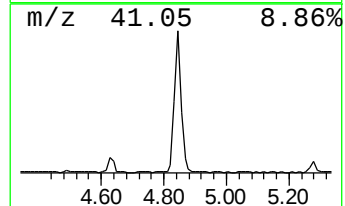
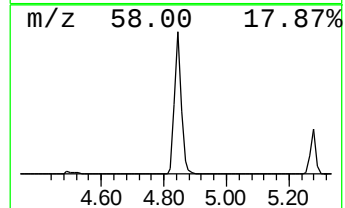
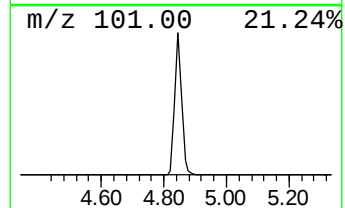
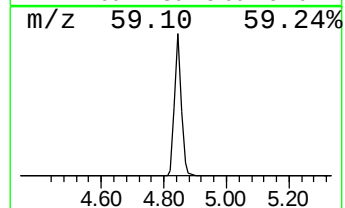
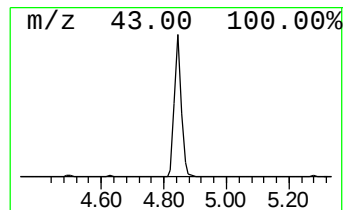
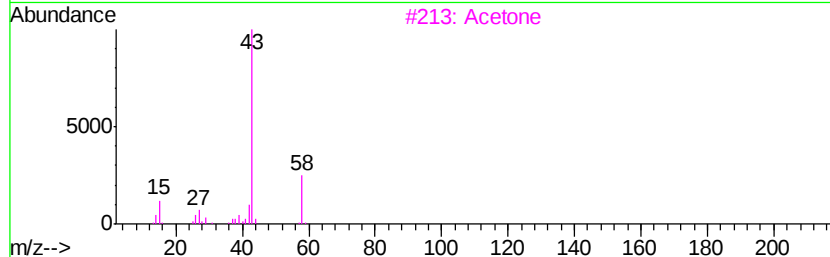
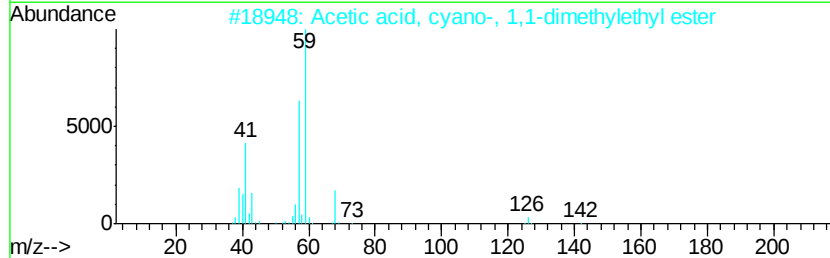
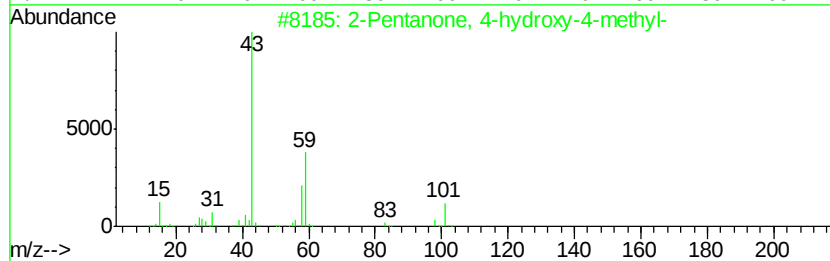
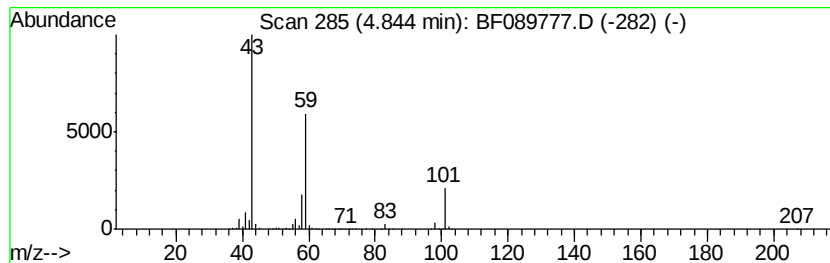
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	23.14 ng	3950090	1,4-Dichlorobenzene-d4	6.70

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23	
3	Acetone	58	C3H6O	000067-64-1	9	
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9	
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	



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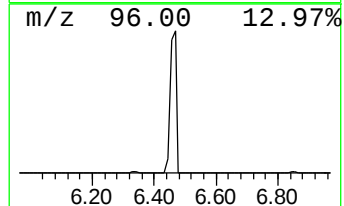
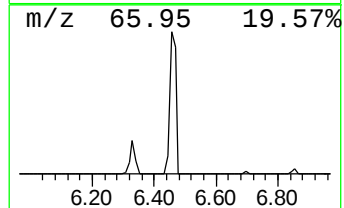
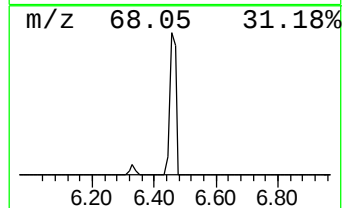
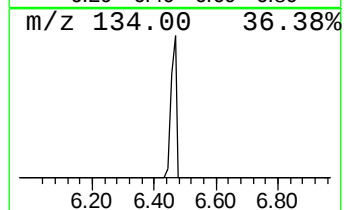
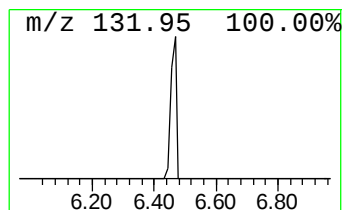
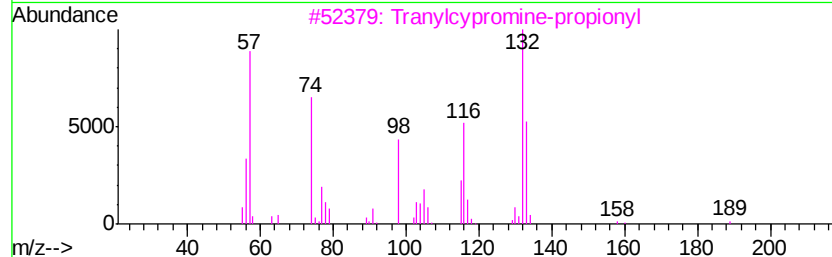
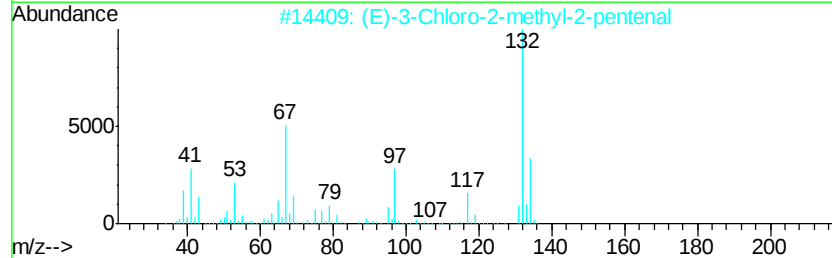
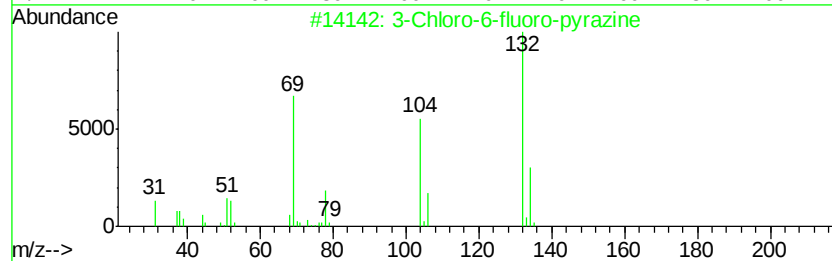
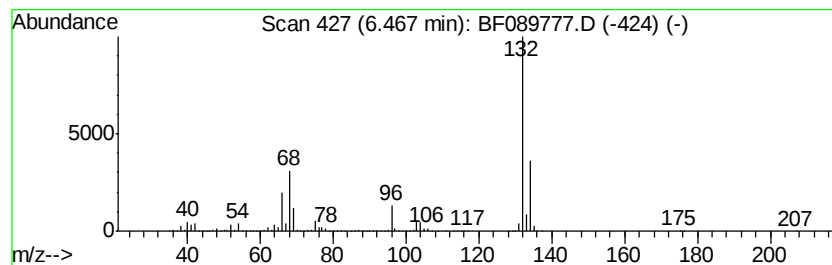
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 unknown6.47 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	78.10 ng	13328600	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	16
4		Amphetaminil	250	C17H18N2	017590-01-1	12
5		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	12



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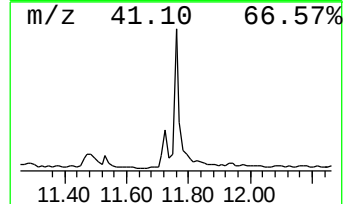
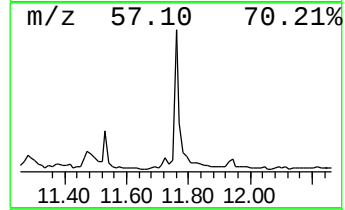
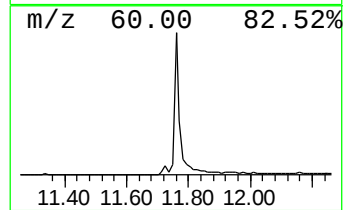
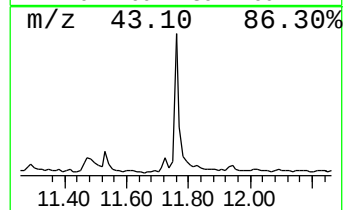
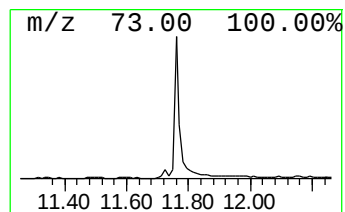
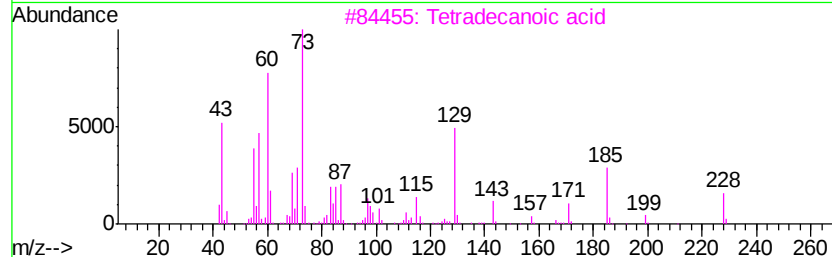
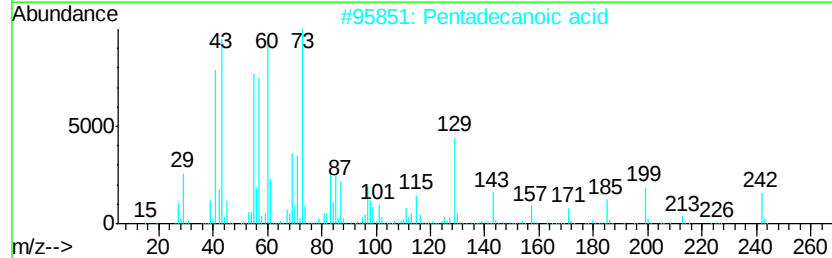
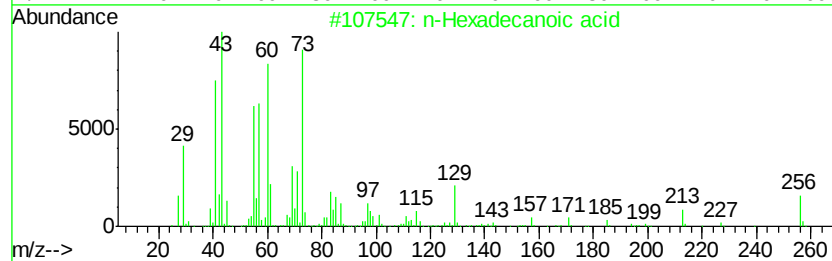
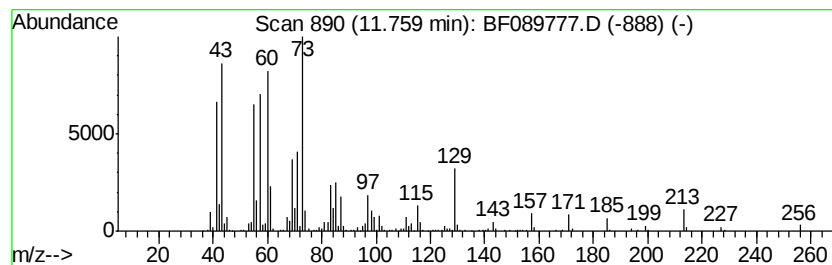
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.76	4.01 ng	1054470	Phenanthrene-d10		11.21
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Tridecanoic acid	214	C13H26O2	000638-53-9	70
5	Silane, trichlorodocosyl-	442	C22H45Cl3Si	007325-84-0	20



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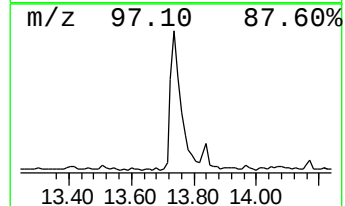
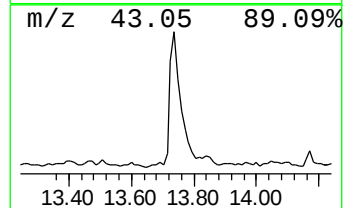
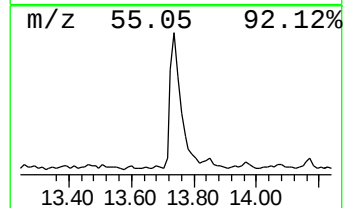
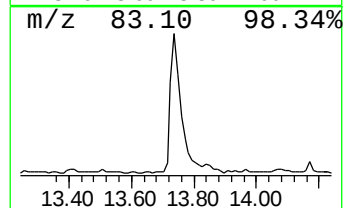
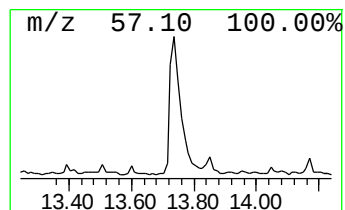
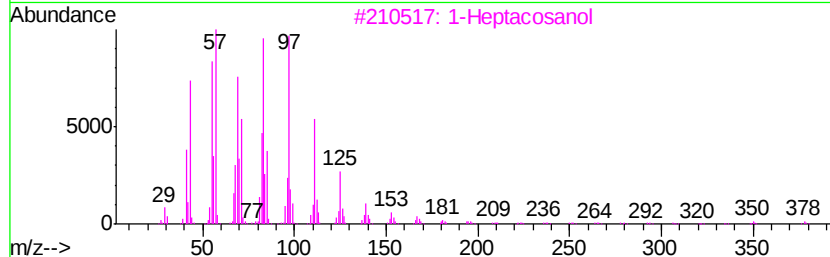
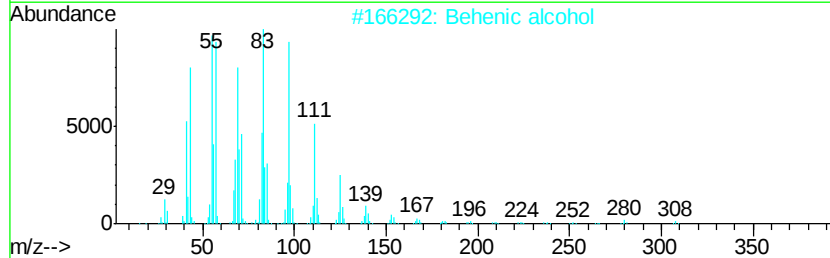
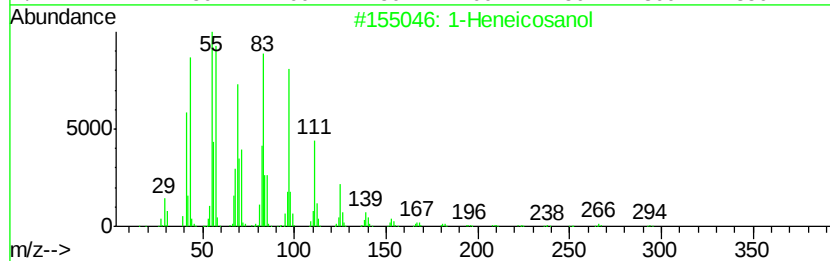
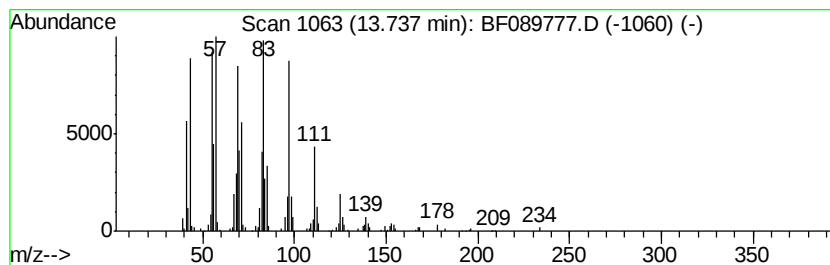
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Peak Number 7 1-Heneicosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.74	3.34 ng	847158	Chrysene-d12	13.84	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	1-Heptacosanol	396	C27H56O	002004-39-9	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91



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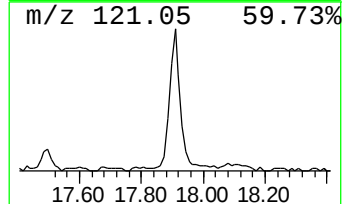
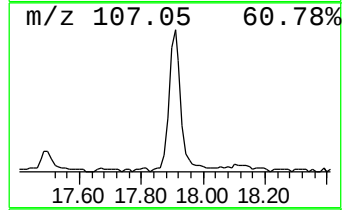
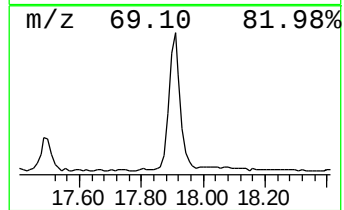
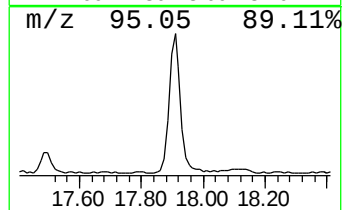
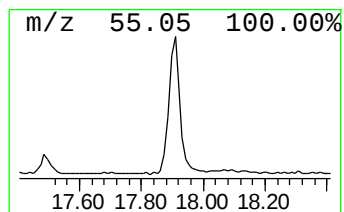
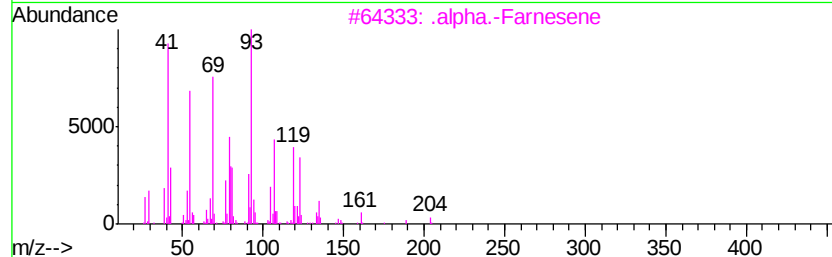
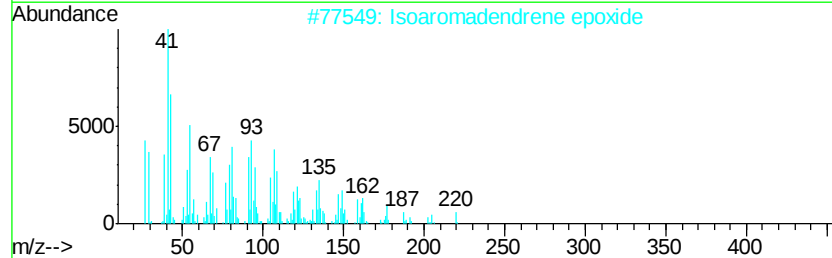
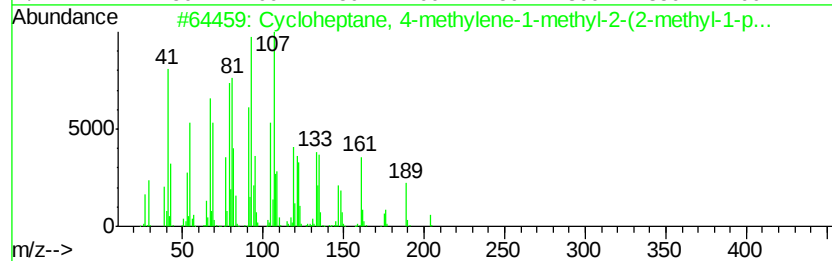
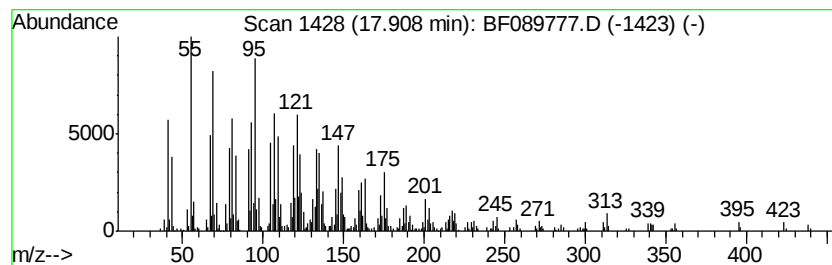
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TIC Library : C:\Database\NIST11.L
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Peak Number 8 Cycloheptane, 4-methylene-1... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.91	8.29 ng	1700100	Perylene-d12	15.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cycloheptane, 4-methylene-1-meth...	204	C15H24	1000159-38-5	68
2		Isoaromadendrene epoxide	220	C15H24O	1000159-36-6	46
3		.alpha.-Farnesene	204	C15H24	000502-61-4	38
4		Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	38
5		5,9-Undecadien-1-yne, 6,10-dimet...	176	C13H20	100451-98-7	25



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TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.84	23.1	ng	3950090	1	6.70	3413430	20.0
unknown6.47	6.47	78.1	ng	13328600	1	6.70	3413430	20.0
n-Hexadecanoic acid	11.76	4.0	ng	1054470	4	11.21	5255180	20.0
1-Heneicosanol	13.74	3.3	ng	847158	5	13.84	5069260	20.0
Cycloheptane, 4-m...	17.91	8.3	ng	1700100	6	15.25	4102790	20.0