

Data Path : Z:\HPCHEM1\BNA F\DATA\BF063017\
 Data File : BF096358.D
 Acq On : 1 Jul 2017 1:28
 Operator : SJ/MA
 Sample : I3930-06
 Misc :
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B2-10-12.5

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-BF062717.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	4.957	483	488	497	rVB	411714	535689	16.00%	1.999%
2	5.375	554	559	562	rBV	3398653	3348058	100.00%	12.493%
3	6.392	726	732	735	rBV	3287363	3293487	98.37%	12.289%
4	6.528	750	755	758	rBV	3297253	3161531	94.43%	11.797%
5	6.757	790	794	798	rBV	1181402	965639	28.84%	3.603%
6	6.916	817	821	824	rVB	2520096	2177542	65.04%	8.125%
7	7.316	884	889	892	rBV	2125283	1954360	58.37%	7.292%
8	7.404	901	904	911	rVB	37781	37274	1.11%	0.139%
9	8.039	1007	1012	1015	rBV	1476112	1230421	36.75%	4.591%
10	9.116	1190	1195	1198	rBV	2669892	2306802	68.90%	8.607%
11	9.504	1256	1261	1264	rBV	382800	341625	10.20%	1.275%
12	9.739	1297	1301	1304	rVB	55645	42816	1.28%	0.160%
13	9.792	1304	1310	1314	rBV	1221199	1032781	30.85%	3.854%
14	10.233	1382	1385	1388	rVB	63405	54104	1.62%	0.202%
15	10.575	1439	1443	1447	rBV	1489747	1288884	38.50%	4.809%
16	10.710	1462	1466	1472	rBV	60132	64447	1.92%	0.240%
17	11.157	1533	1542	1544	rBV2	34358	40561	1.21%	0.151%
18	11.269	1558	1561	1564	rBV	948359	833051	24.88%	3.108%
19	11.504	1596	1601	1606	rBV3	34372	35221	1.05%	0.131%
20	11.804	1649	1652	1662	rBV3	136318	149276	4.46%	0.557%
21	12.480	1763	1767	1770	rBV	34187	37446	1.12%	0.140%
22	12.592	1782	1786	1792	rBV	32835	42177	1.26%	0.157%
23	12.857	1826	1831	1834	rBV	1843698	1617747	48.32%	6.036%
24	13.339	1908	1913	1917	rBV	66713	74557	2.23%	0.278%
25	13.557	1946	1950	1954	rVB	208944	186888	5.58%	0.697%
26	13.757	1980	1984	1991	rBV	286973	288871	8.63%	1.078%
27	13.904	2004	2009	2012	rBV	901052	924790	27.62%	3.451%
28	14.204	2057	2060	2065	rBV2	60343	62558	1.87%	0.233%
29	14.392	2089	2092	2093	rBV	51015	53102	1.59%	0.198%
30	15.321	2246	2250	2255	rVB	519726	618716	18.48%	2.309%

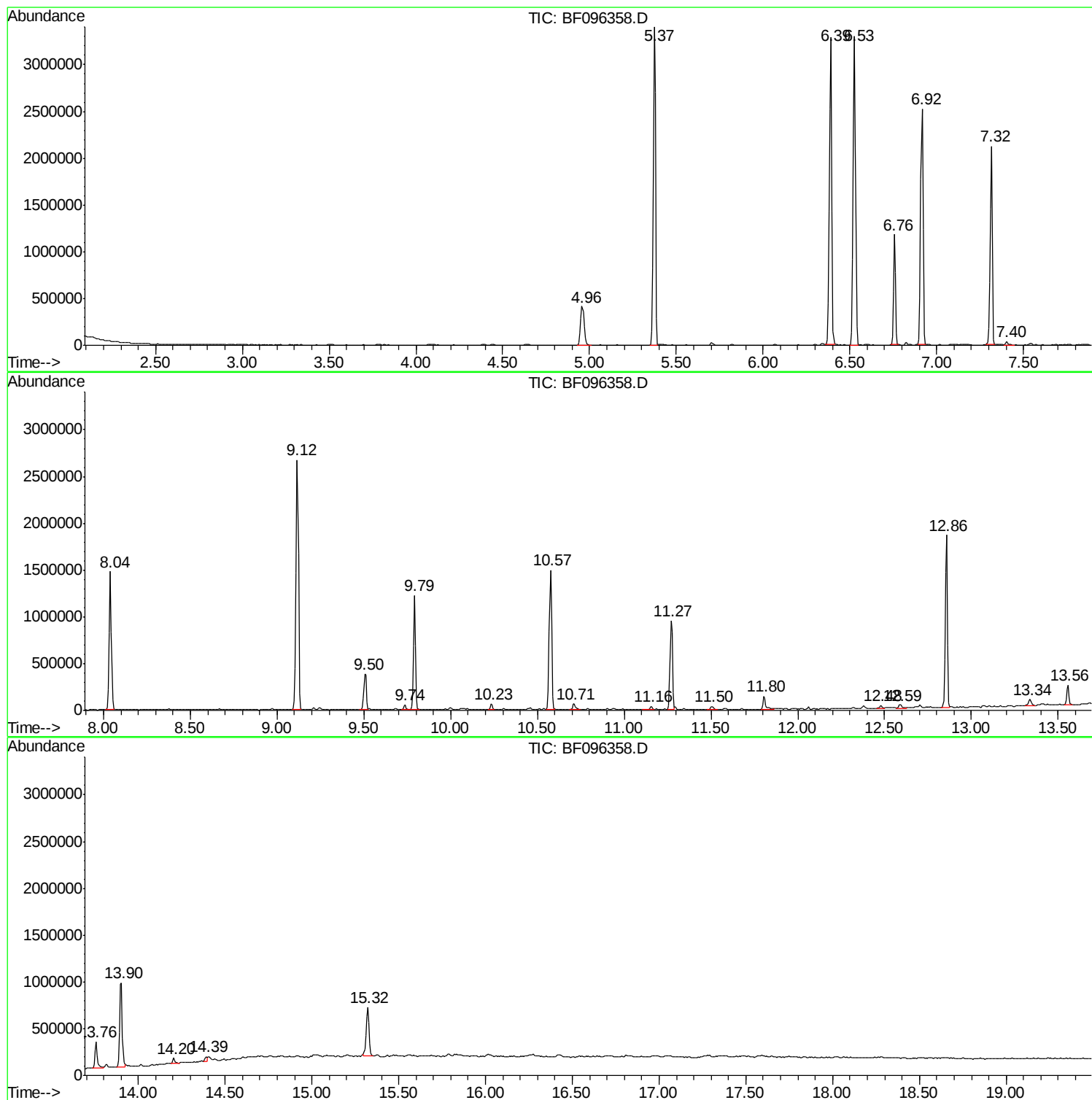
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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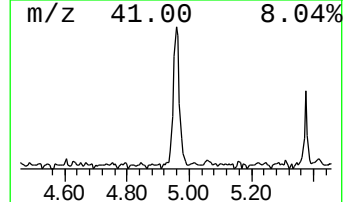
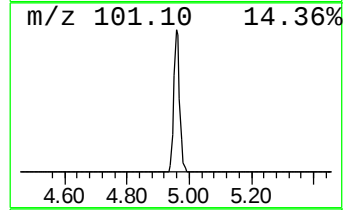
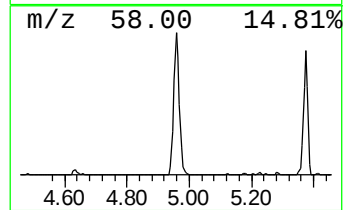
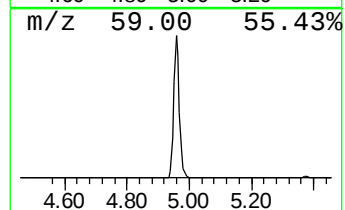
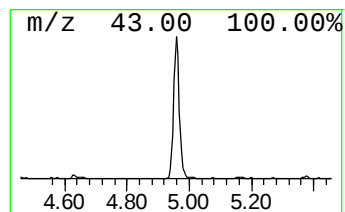
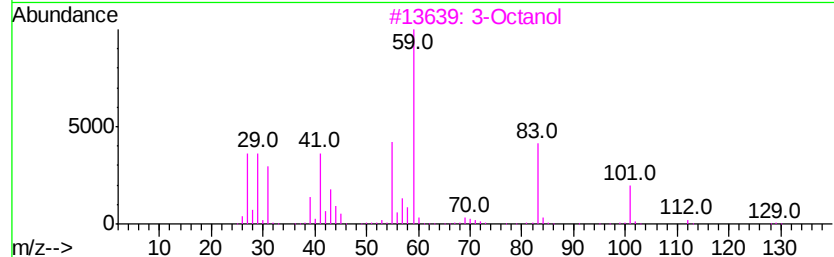
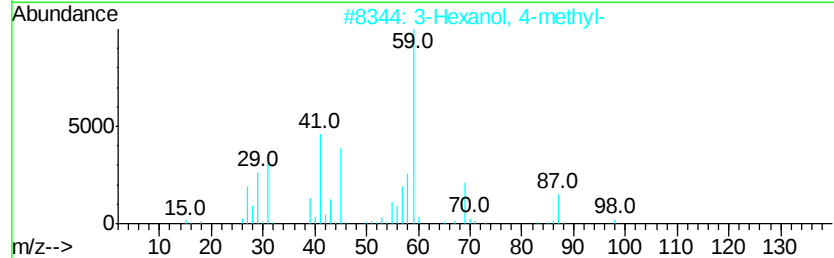
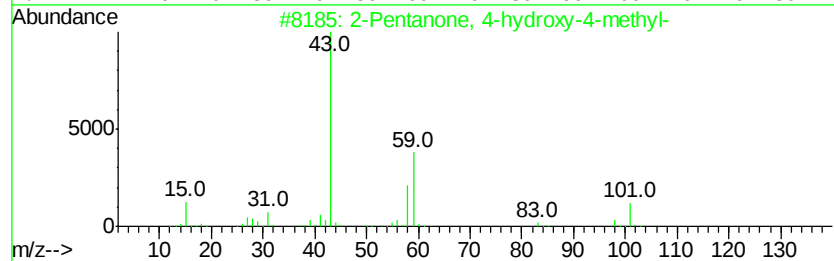
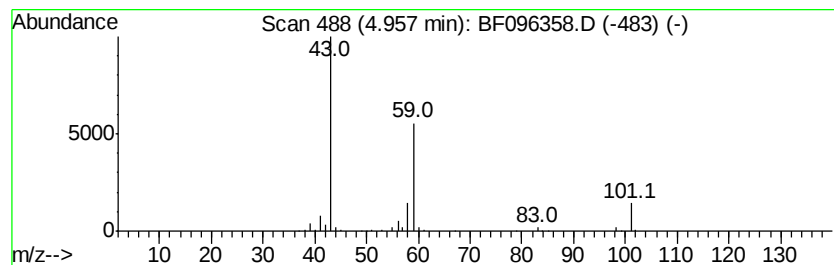
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	11.10 ng	535689	1,4-Dichlorobenzene-d4	6.76

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			3-Octanol	130	C8H18O	000589-98-0	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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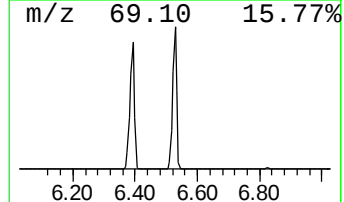
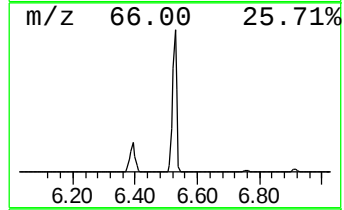
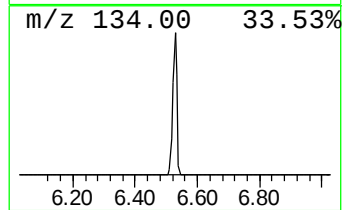
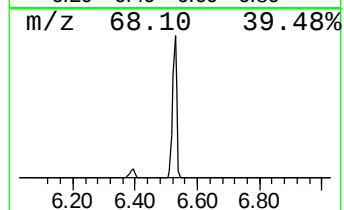
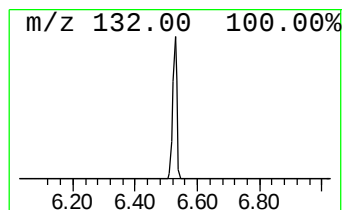
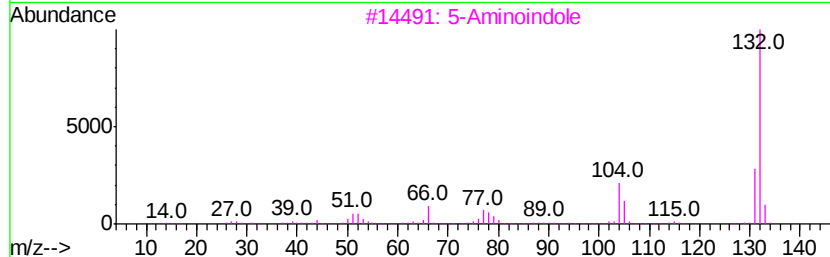
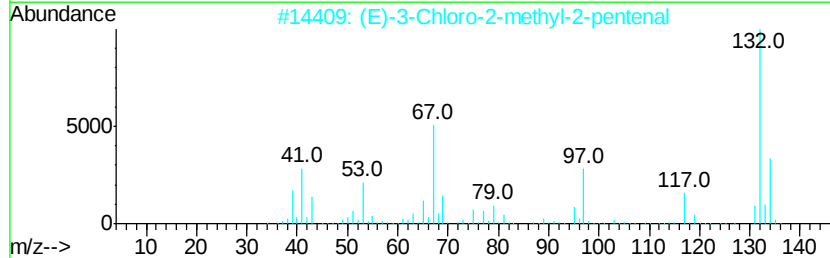
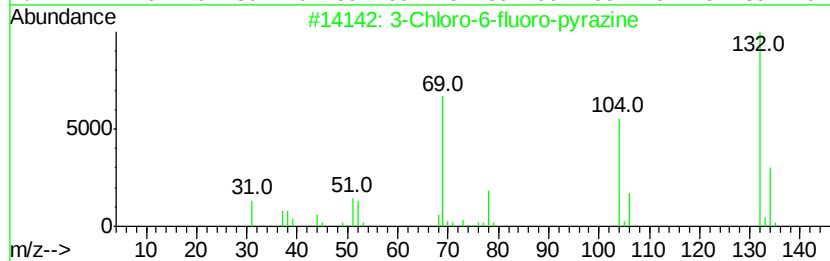
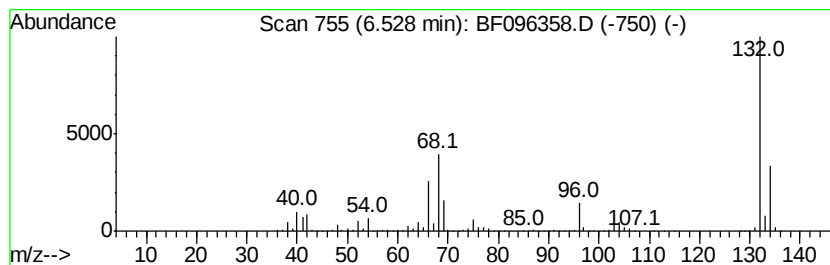
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Peak Number 2 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	65.48 ng	3161530	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Amphetaminil	250	C17H18N2	017590-01-1	10
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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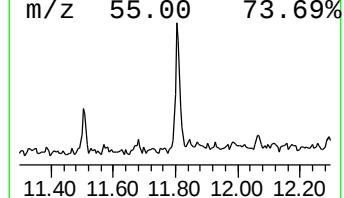
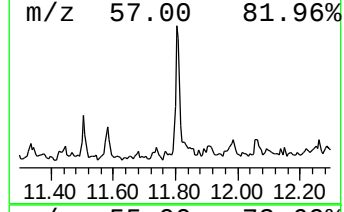
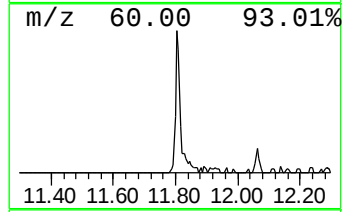
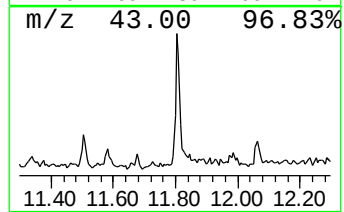
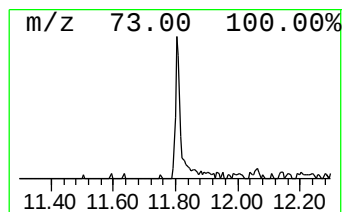
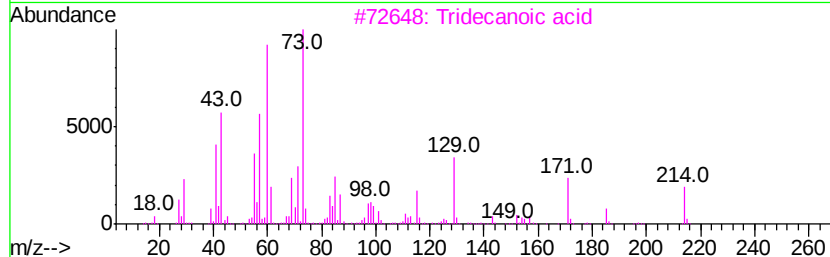
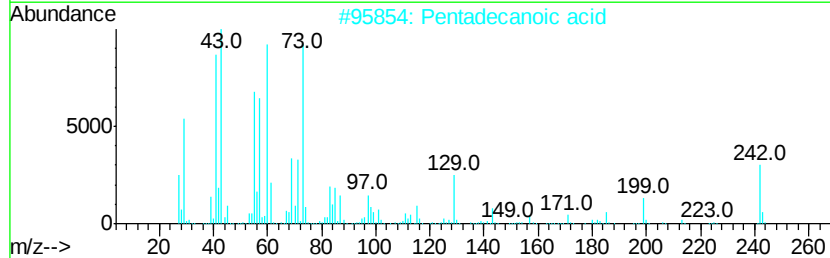
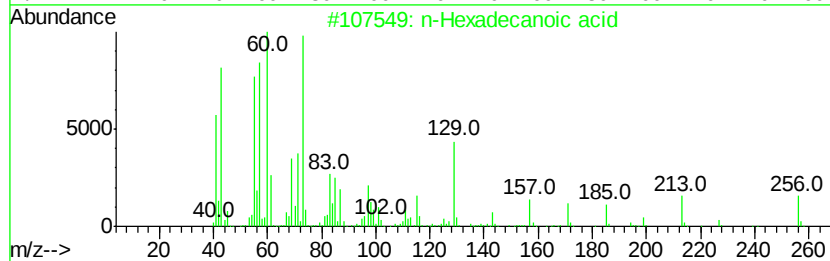
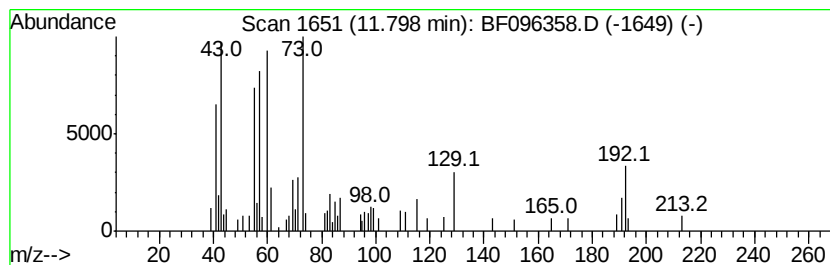
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.80	3.58 ng	149276	Phenanthrene-d10	11.27

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			Tridecanoic acid	214	C13H26O2	000638-53-9	80
4			Undecanoic acid	186	C11H22O2	000112-37-8	72
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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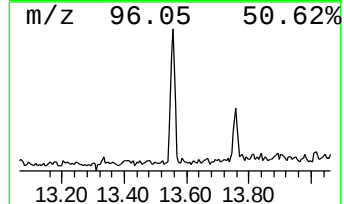
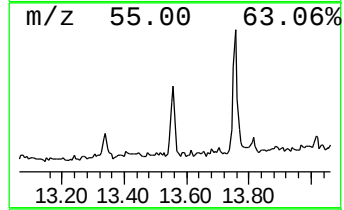
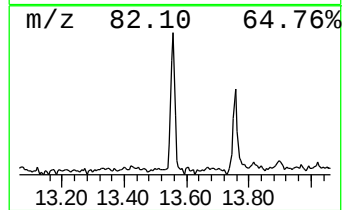
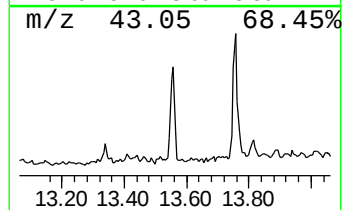
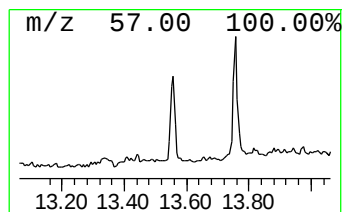
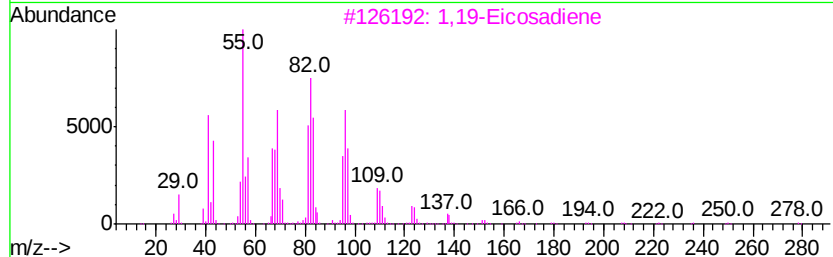
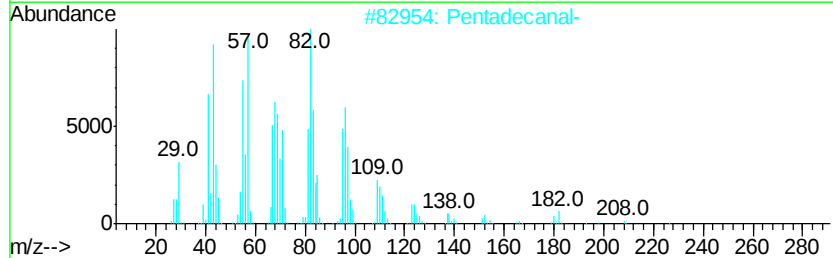
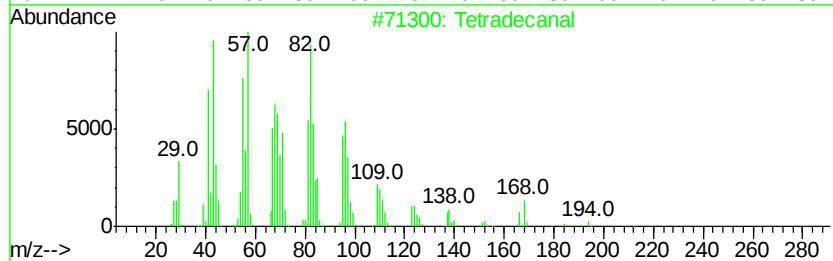
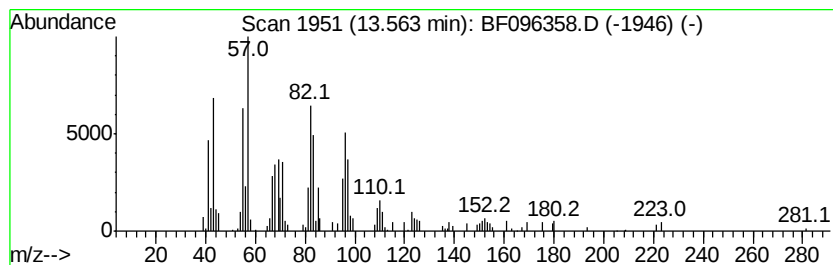
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Peak Number 5 Tetradecanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.56	4.04 ng	186888	Chrysene-d12		13.90
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanal	212	C14H28O	000124-25-4	91
2	Pentadecanal-	226	C15H30O	002765-11-9	91
3	1,19-Eicosadiene	278	C20H38	014811-95-1	81
4	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	76
5	18-Nonadecen-1-ol	282	C19H38O	1000142-89-2	74



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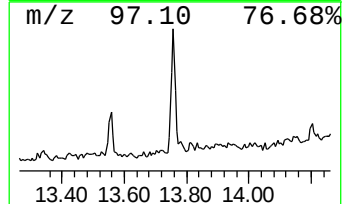
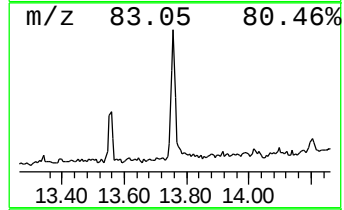
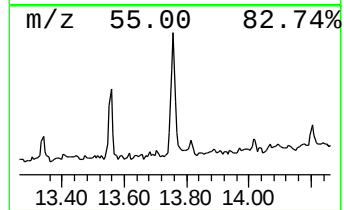
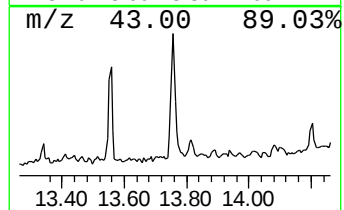
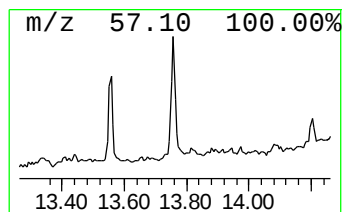
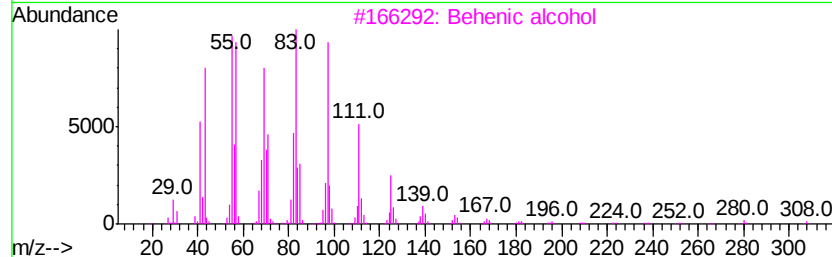
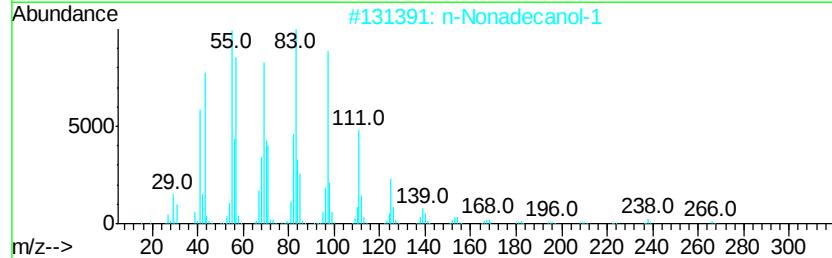
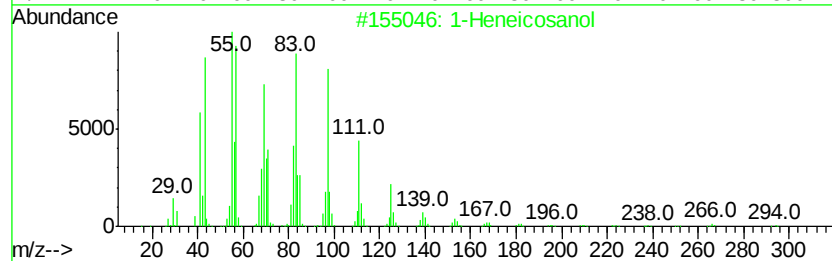
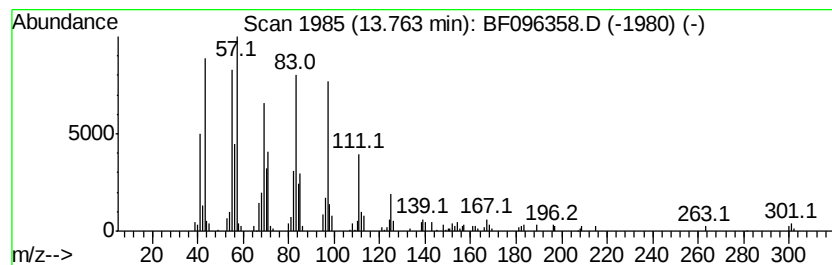
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Peak Number 6 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	6.25 ng	288871	Chrysene-d12	13.90

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol		312	C21H44O	015594-90-8	95
2	n-Nonadecanol-1		284	C19H40O	001454-84-8	93
3	Behenic alcohol		326	C22H46O	000661-19-8	93
4	Trifluoroacetoxy hexadecane		338	C18H33F3O2	006222-03-3	91
5	1-Octadecanol		270	C18H38O	000112-92-5	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.96	11.1	ng	535689	1	6.76	965639	20.0
unknown6.53	6.53	65.5	ng	3161530	1	6.76	965639	20.0
n-Hexadecanoic acid	11.80	3.6	ng	149276	4	11.27	833051	20.0
Tetradecanal	13.56	4.0	ng	186888	5	13.90	924790	20.0
1-Heneicosanol	13.76	6.3	ng	288871	5	13.90	924790	20.0