

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040618\
 Data File : BF104348.D
 Acq On : 7 Apr 2018 10:17
 Operator : JU/SJ
 Sample : J2255-03
 Misc :
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 040418-JETB-E-D-S

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-BF040618.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	4.998	491	495	502	rVB	165346	167895	3.93%	0.670%
2	5.404	559	564	567	rBV	1381974	1182297	27.66%	4.721%
3	6.416	732	736	739	rBV	874931	710764	16.63%	2.838%
4	6.569	757	762	765	rBV	2438376	2205146	51.58%	8.805%
5	6.804	798	802	805	rBV	1042287	871962	20.40%	3.482%
6	6.963	824	829	832	rBV	3117809	2992292	70.00%	11.949%
7	7.369	892	898	901	rBV	2374147	2477048	57.94%	9.891%
8	8.086	1016	1020	1023	rBV	1440867	1153190	26.98%	4.605%
9	9.169	1198	1204	1207	rBV	4030367	4274844	100.00%	17.070%
10	9.557	1266	1270	1273	rBV	143891	130655	3.06%	0.522%
11	9.769	1303	1306	1310	rVB	77871	65450	1.53%	0.261%
12	9.839	1313	1318	1322	rVB	1389127	1252439	29.30%	5.001%
13	10.275	1384	1392	1394	rBV2	84245	80711	1.89%	0.322%
14	10.627	1447	1452	1455	rBV	1787250	1547143	36.19%	6.178%
15	10.745	1469	1472	1480	rVB	65558	62957	1.47%	0.251%
16	11.327	1567	1571	1574	rBV	1159991	983860	23.02%	3.929%
17	12.739	1808	1811	1814	rBV	139796	102858	2.41%	0.411%
18	12.921	1837	1842	1845	rBV	3084708	2964654	69.35%	11.838%
19	13.445	1928	1931	1934	rBV	81411	64600	1.51%	0.258%
20	13.810	1990	1993	2004	rBV	197001	208429	4.88%	0.832%
21	13.968	2016	2020	2023	rBV	963315	815776	19.08%	3.257%
22	15.427	2263	2268	2272	rBV	610699	728065	17.03%	2.907%

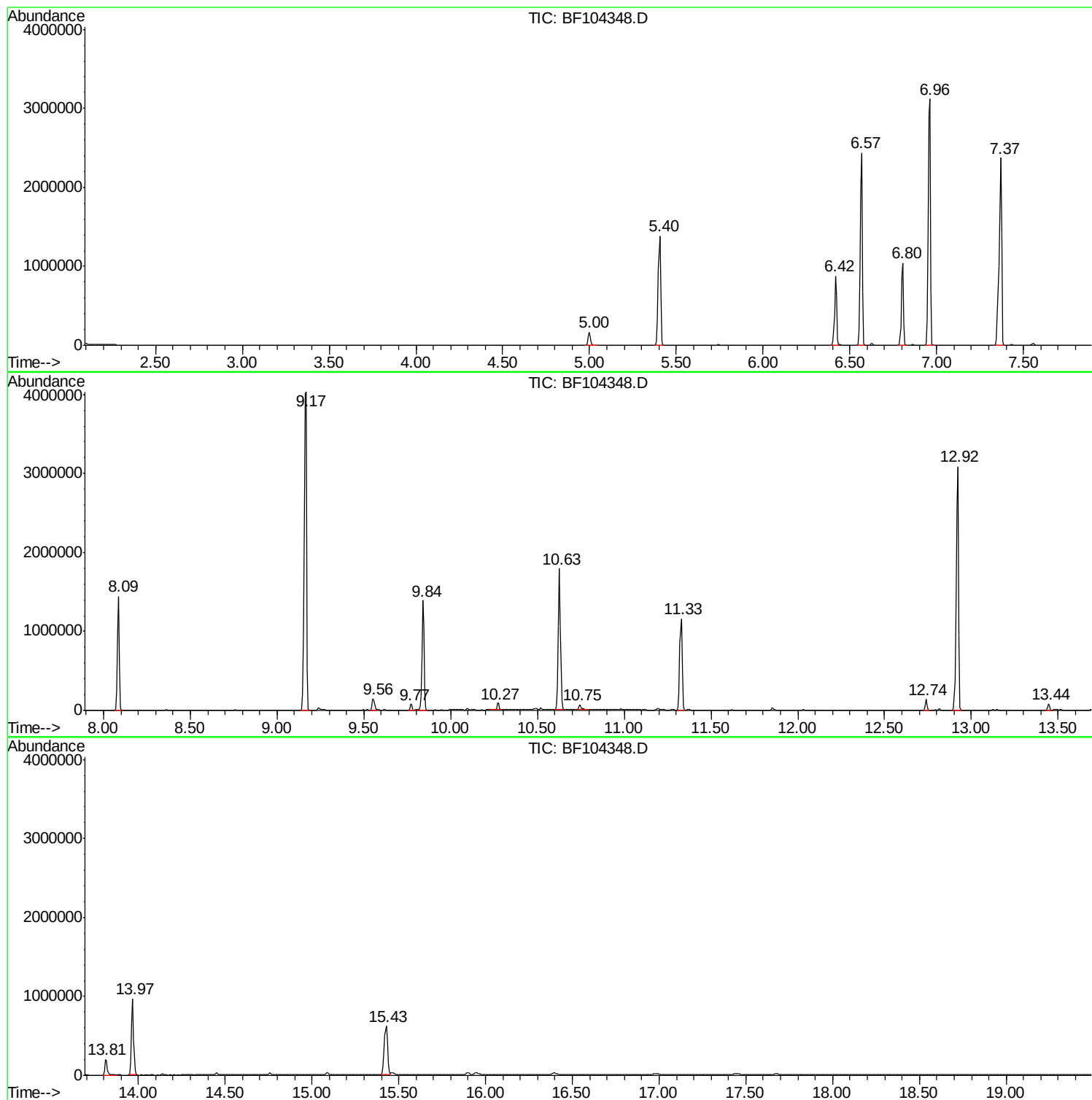
Sum of corrected areas: 25043035

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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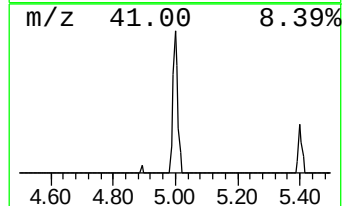
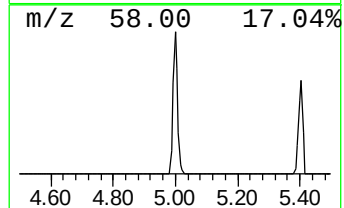
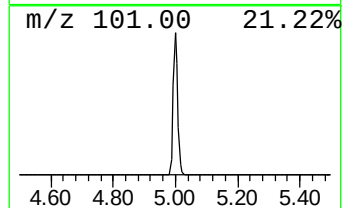
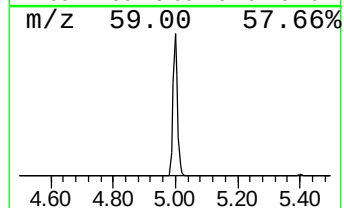
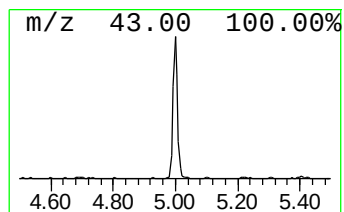
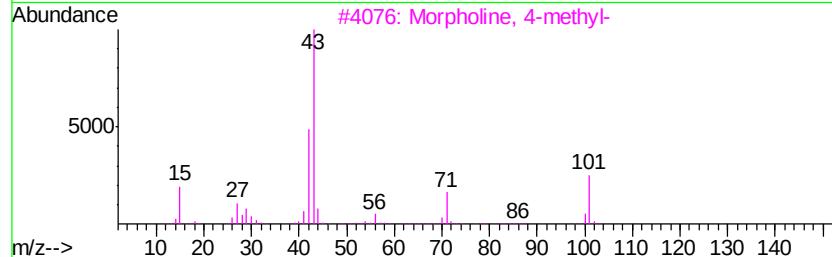
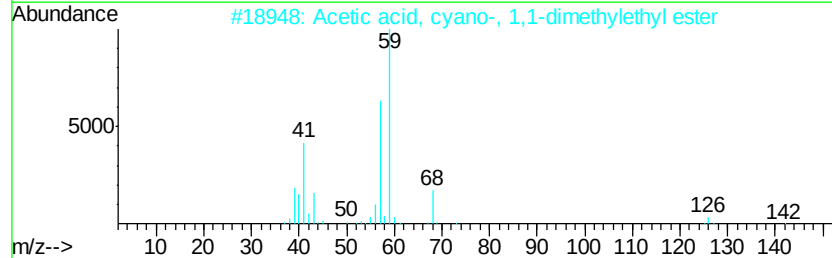
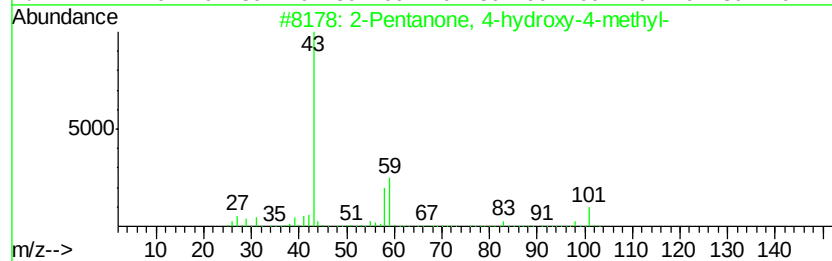
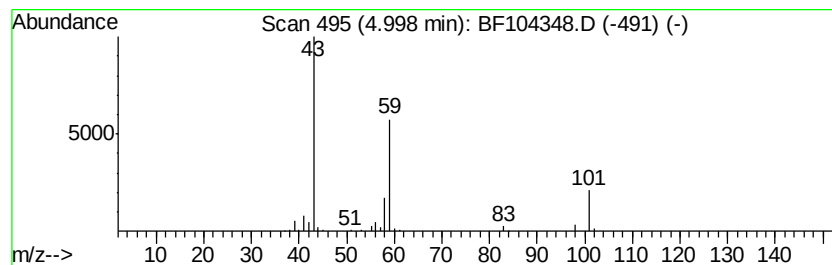
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	3.85 ng	167895	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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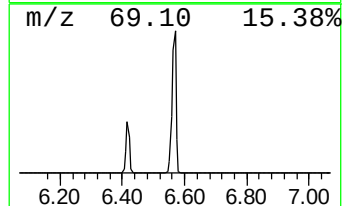
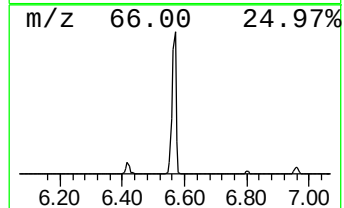
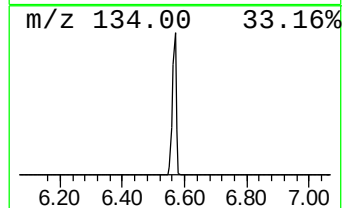
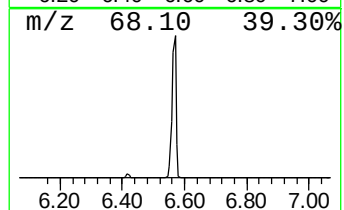
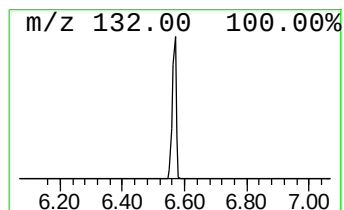
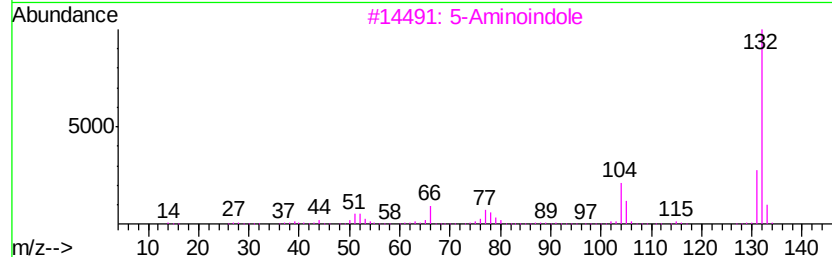
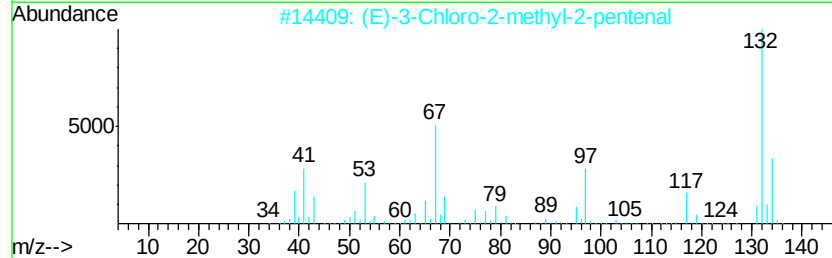
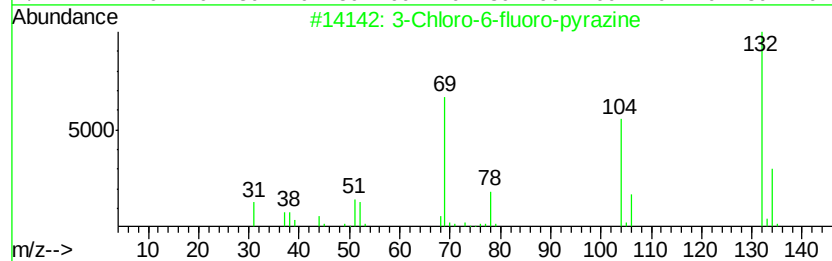
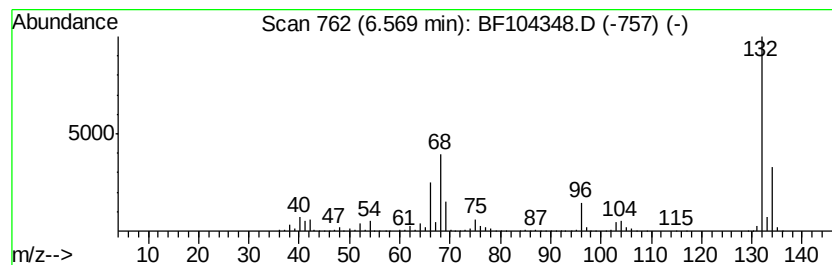
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Peak Number 2 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	50.58 ng	2205150	1,4-Dichlorobenzene-d4	6.80

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	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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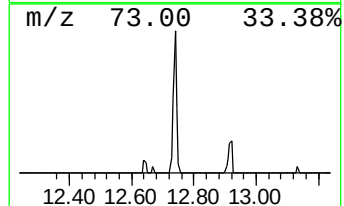
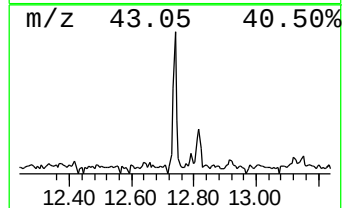
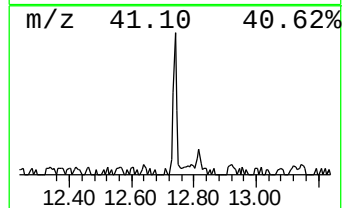
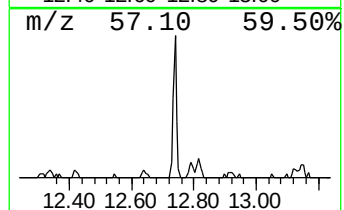
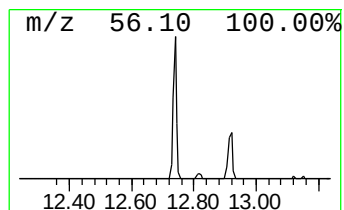
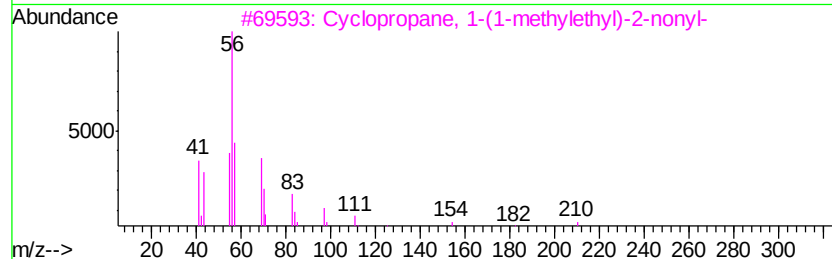
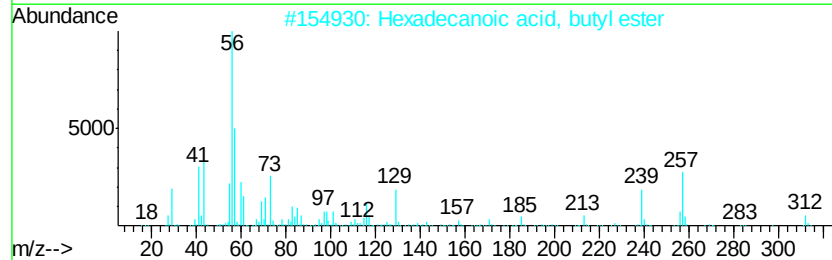
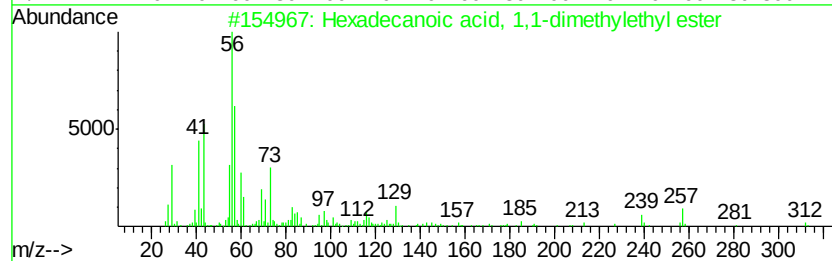
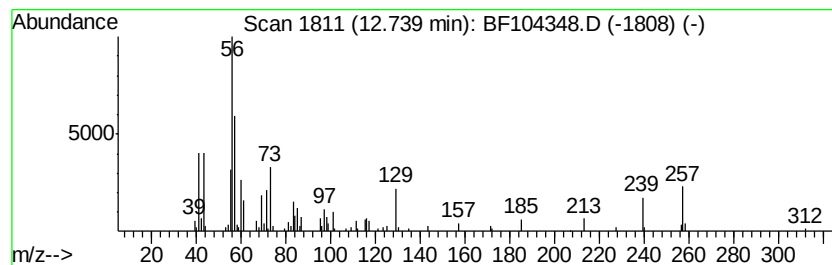
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Peak Number 4 Hexadecanoic acid, 1,1-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.74	2.52 ng	102858	Chrysene-d12	13.97	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	96
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	95
3	Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	35
4	Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	30
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	30



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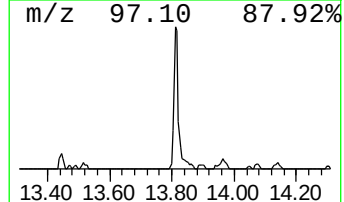
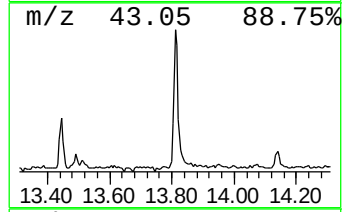
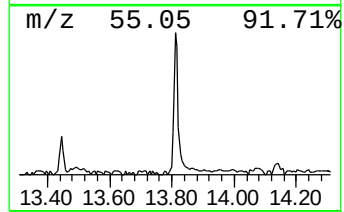
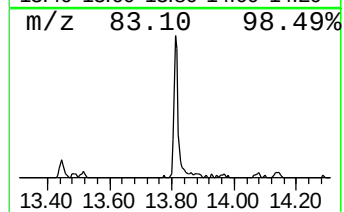
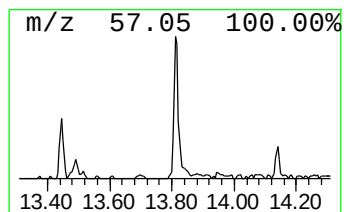
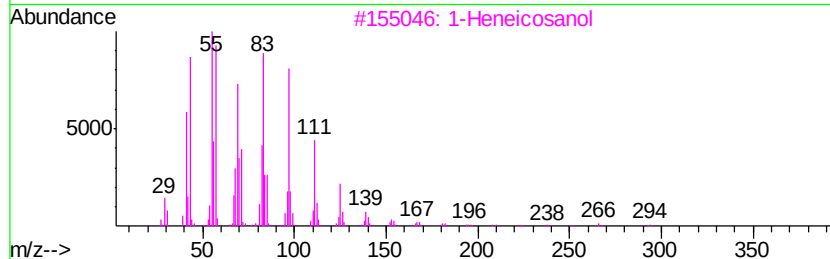
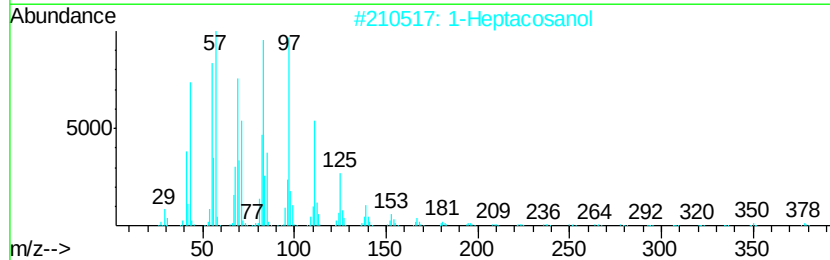
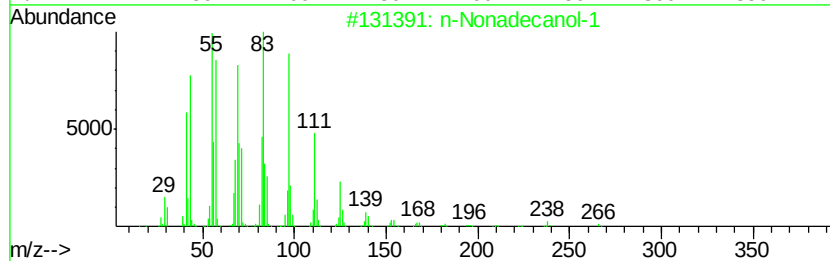
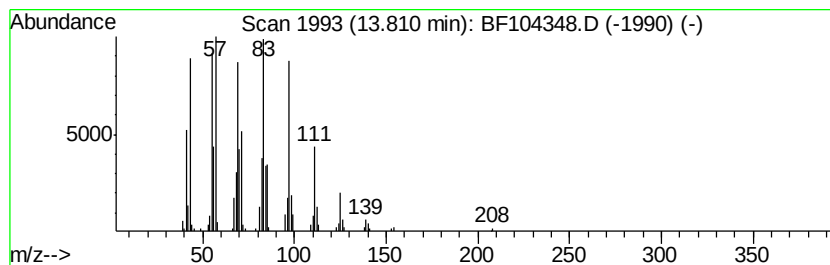
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Peak Number 5 n-Nonadecanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.81	5.11 ng	208429	Chrysene-d12	13.97	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2	1-Heptacosanol	396	C27H56O	002004-39-9	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.00	3.9	ng	167895	1	6.80	871962	20.0
unknown6.57	6.57	50.6	ng	2205150	1	6.80	871962	20.0
Hexadecanoic acid...	12.74	2.5	ng	102858	5	13.97	815776	20.0
n-Nonadecanol-1	13.81	5.1	ng	208429	5	13.97	815776	20.0