

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060617\
 Data File : BF095722.D
 Acq On : 6 Jun 2017 22:08
 Operator : SJ/MA
 Sample : I3478-13
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 155-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-BF060517.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	1.804	34	37	50	rVB4	12445	27795	1.22%	0.157%
2	4.604	509	513	529	rBV2	58541	170956	7.48%	0.966%
3	5.275	623	627	657	rBV	1082158	1856222	81.23%	10.488%
4	6.939	905	910	922	rBV	1201225	1805209	79.00%	10.200%
5	7.039	922	927	941	rVB	1492454	2075942	90.85%	11.730%
6	7.380	981	985	999	rVB	355955	465397	20.37%	2.630%
7	7.622	1020	1026	1046	rBV	1155244	1566033	68.53%	8.849%
8	8.298	1136	1141	1163	rBV	826114	1153350	50.47%	6.517%
9	9.410	1326	1330	1343	rBV	476522	625358	27.37%	3.534%
10	11.198	1627	1634	1646	rBV	1764083	2285030	100.00%	12.911%
11	11.886	1747	1751	1759	rBV	126812	148842	6.51%	0.841%
12	12.233	1805	1810	1816	rBV2	525849	643322	28.15%	3.635%
13	13.092	1950	1956	1961	rBV2	22998	29389	1.29%	0.166%
14	13.527	2025	2030	2046	rBV	805405	1062027	46.48%	6.001%
15	13.862	2082	2087	2097	rBV	23801	38406	1.68%	0.217%
16	14.627	2213	2217	2223	rBV	447153	553524	24.22%	3.128%
17	15.645	2386	2390	2399	rBV	89736	107093	4.69%	0.605%
18	16.450	2519	2527	2533	rBV	48639	65219	2.85%	0.369%
19	16.750	2572	2578	2586	rBV2	65019	99194	4.34%	0.560%
20	17.003	2615	2621	2624	rBV	1401567	1632417	71.44%	9.224%
21	18.250	2829	2833	2843	rBV	110804	166295	7.28%	0.940%
22	18.339	2843	2848	2854	rBV	390206	466512	20.42%	2.636%
23	19.056	2966	2970	2978	rVB2	22648	33609	1.47%	0.190%
24	19.491	3040	3044	3049	rVB	22584	27447	1.20%	0.155%
25	19.615	3062	3065	3069	rBV	25545	34680	1.52%	0.196%
26	19.797	3089	3096	3102	rBV6	25353	57145	2.50%	0.323%
27	19.962	3120	3124	3127	rVV	24697	25898	1.13%	0.146%
28	20.003	3127	3131	3142	rVV	322219	415373	18.18%	2.347%
29	20.456	3205	3208	3211	rBV2	23058	29159	1.28%	0.165%
30	20.497	3211	3215	3219	rVV7	17807	30926	1.35%	0.175%

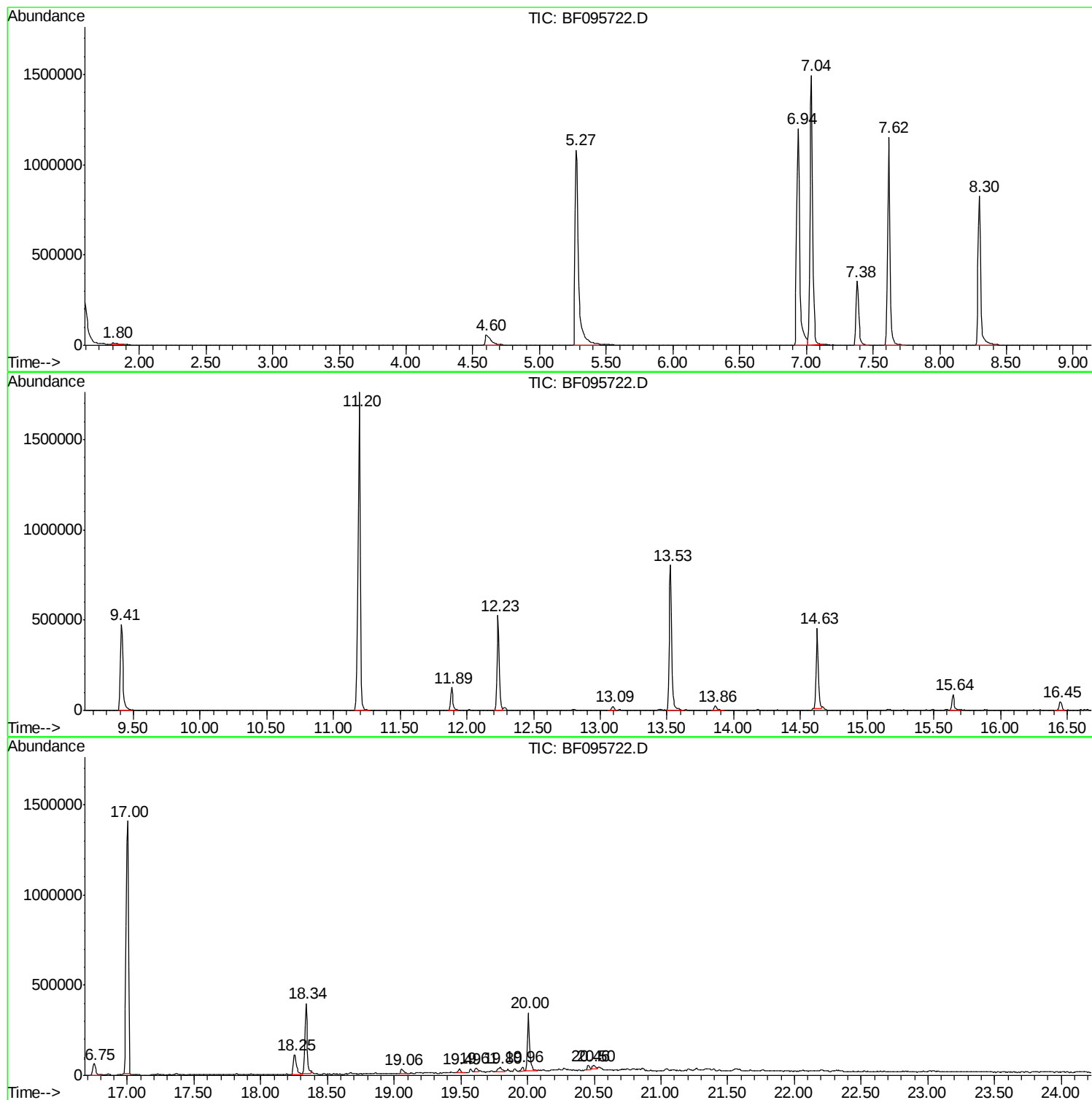
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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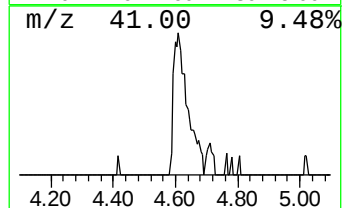
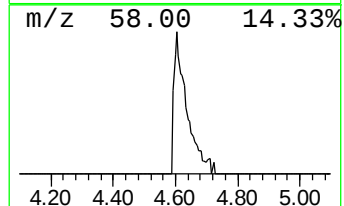
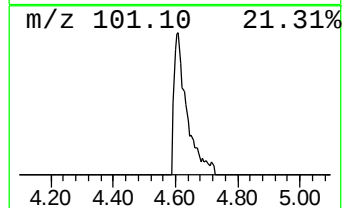
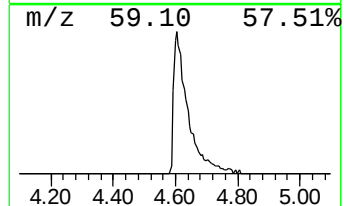
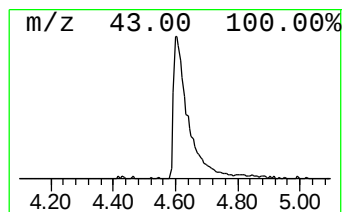
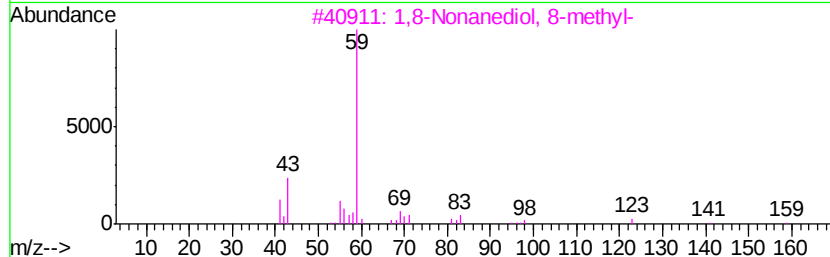
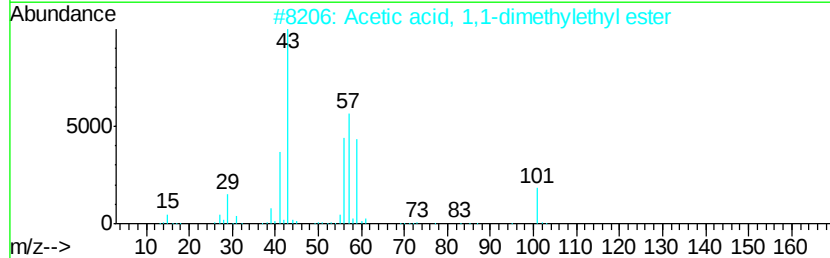
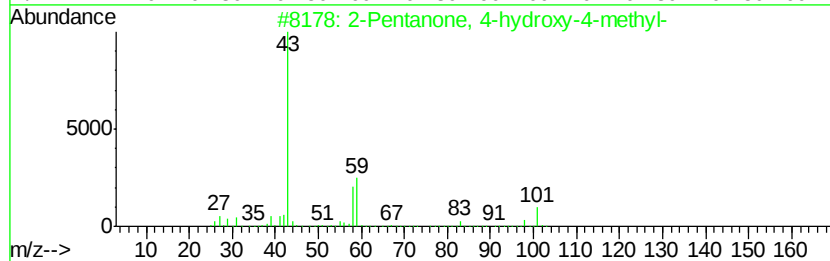
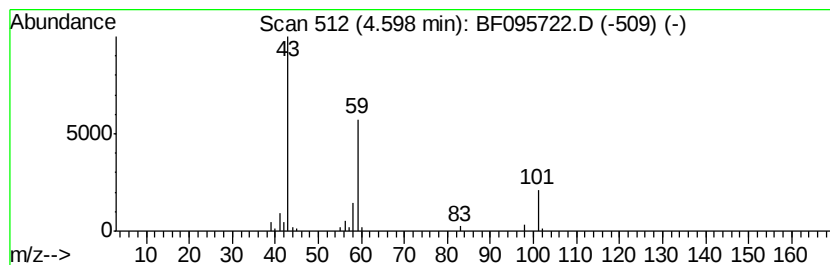
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.60	7.35 ng	170956	1,4-Dichlorobenzene-d4	7.38

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	38
3			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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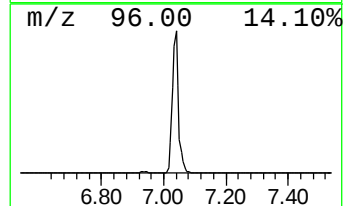
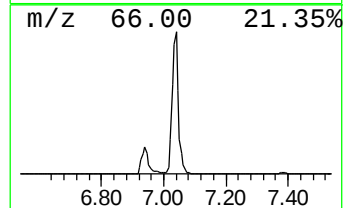
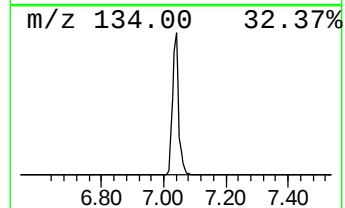
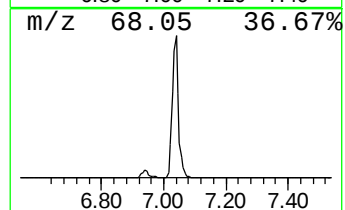
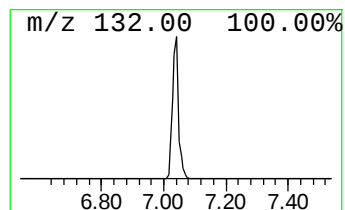
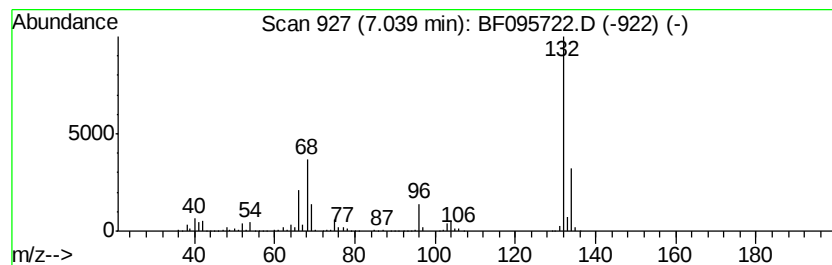
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.04	89.21 ng	2075940	1,4-Dichlorobenzene-d4	7.38

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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9



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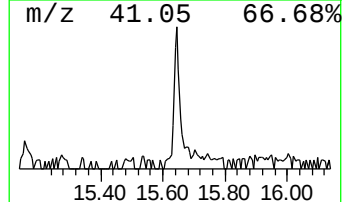
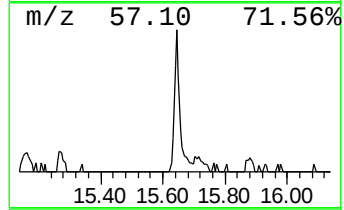
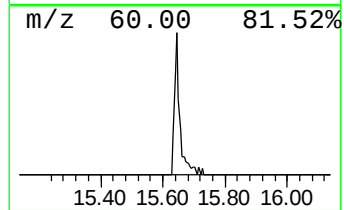
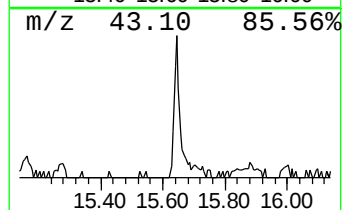
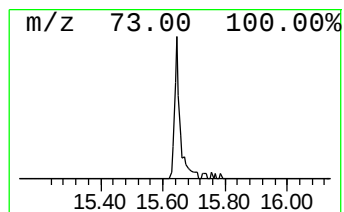
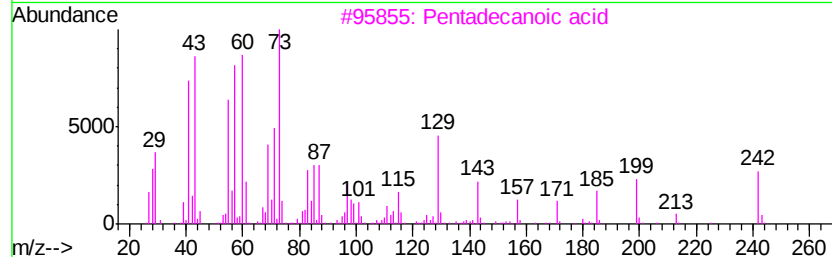
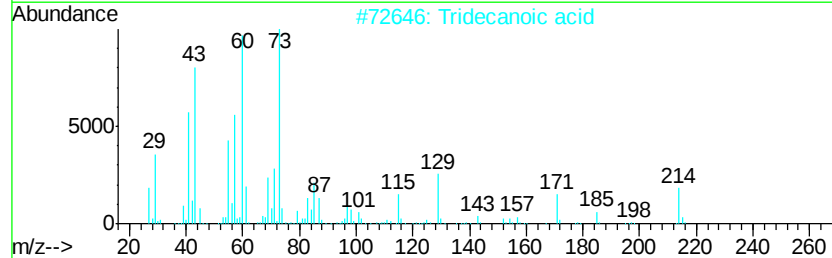
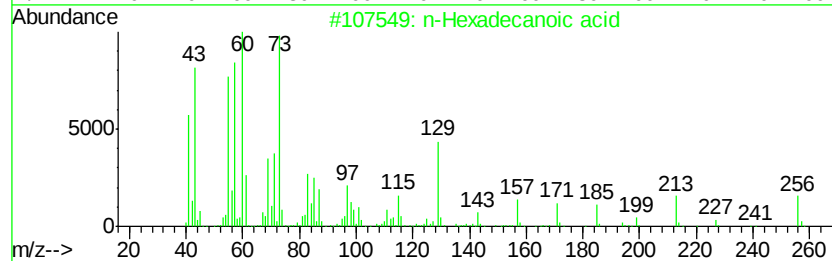
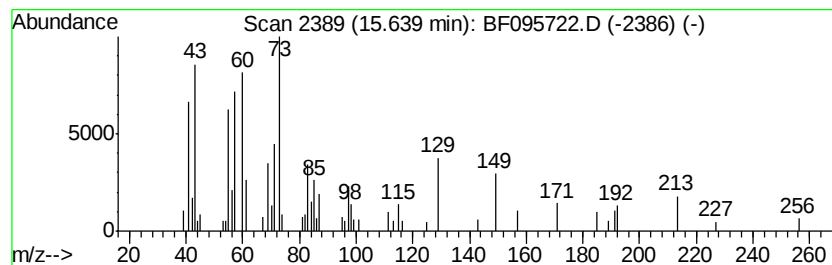
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.64	3.87 ng	107093	Phenanthrene-d10	14.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Tridecanoic acid	214	C13H26O2	000638-53-9	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5		Dodecanoic acid	200	C12H24O2	000143-07-7	59



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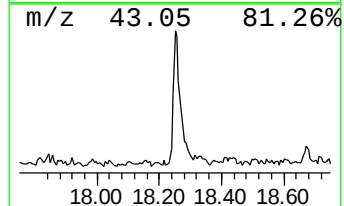
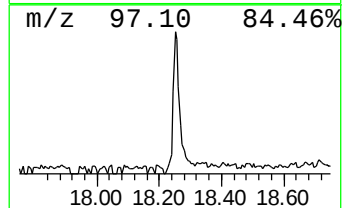
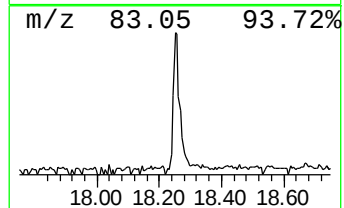
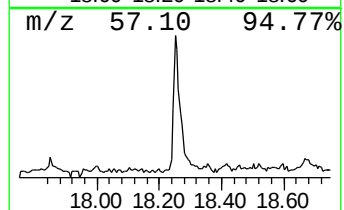
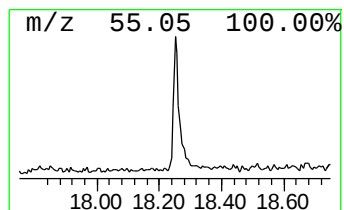
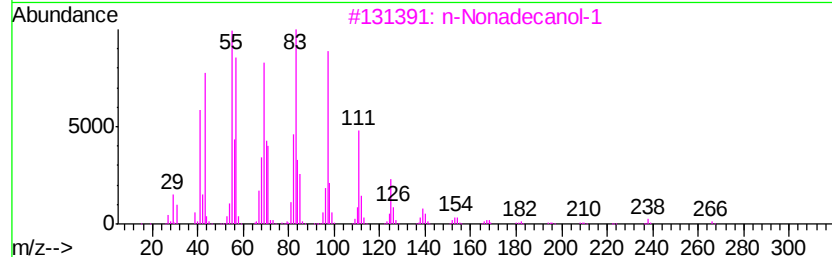
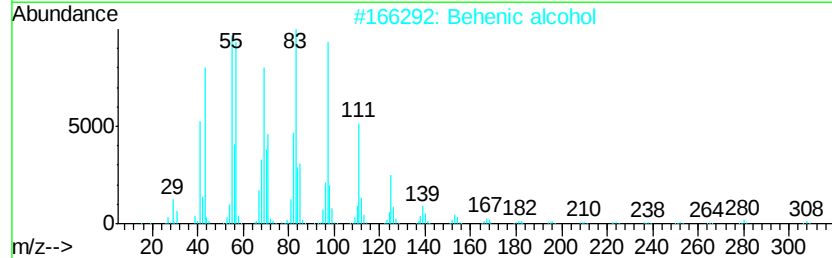
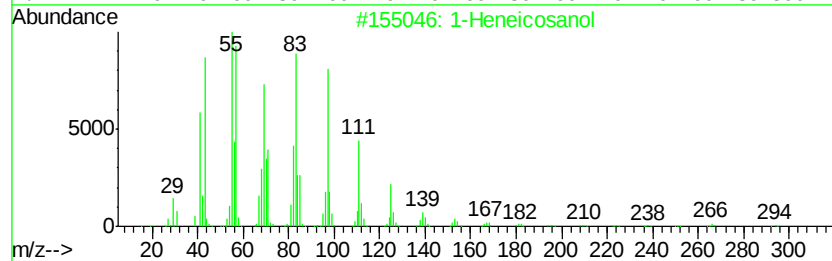
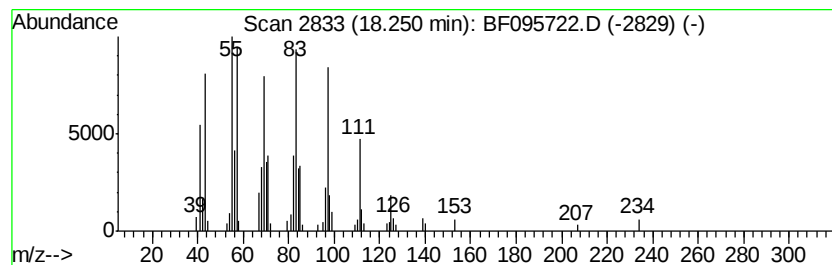
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Peak Number 6 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.25	7.13 ng	166295	Chrysene-d12	18.34
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	94
3	n-Nonadecanol-1	284 C19H40O	001454-84-8	94
4	n-Tetracosanol-1	354 C24H50O	000506-51-4	94
5	n-Heptadecanol-1	256 C17H36O	001454-85-9	91



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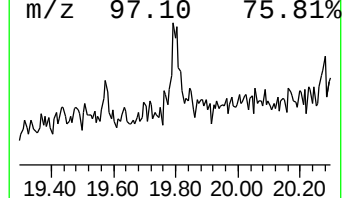
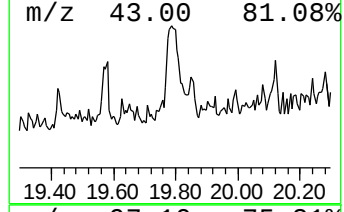
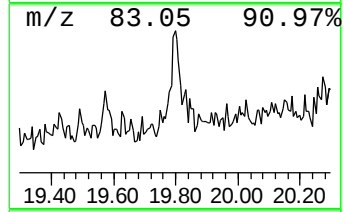
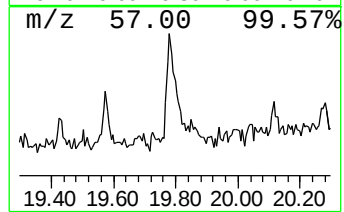
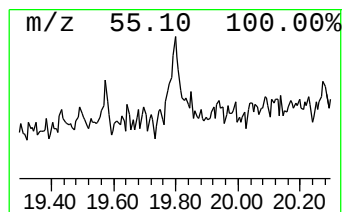
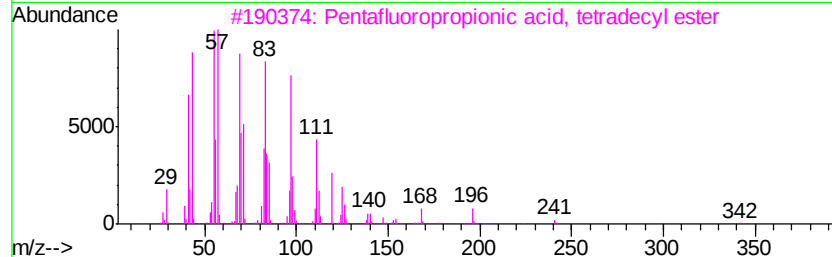
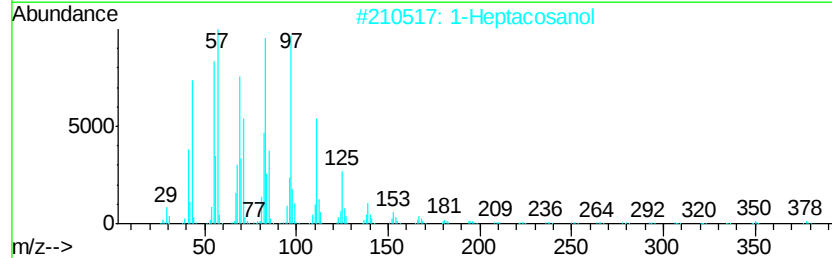
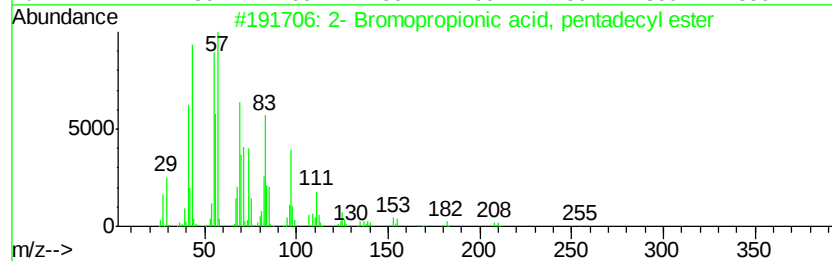
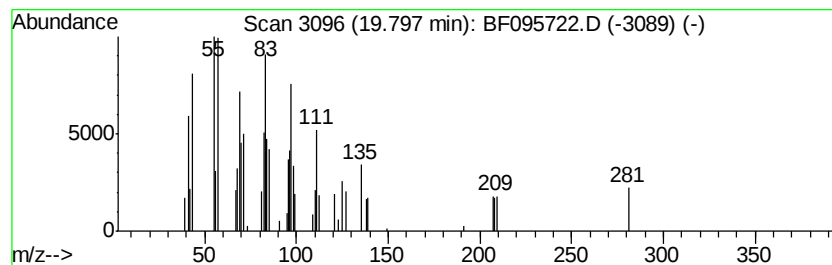
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Peak Number 7 2- Bromopropionic acid, pen... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.80	2.75 ng	57145	Perylene-d12	20.00

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-	Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	62	
2	1-	Heptacosanol	396	C27H56O	002004-39-9	60	
3		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	58	
4	2-	Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	58	
5		11-Tricosene	322	C23H46	052078-56-5	58	



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.60	7.3	ng	170956	1	7.38	465397	20.0
unknown7.04	7.04	89.2	ng	2075940	1	7.38	465397	20.0
n-Hexadecanoic acid	15.64	3.9	ng	107093	4	14.63	553524	20.0
1-Heneicosanol	18.25	7.1	ng	166295	5	18.34	466512	20.0
2- Bromopropionic...	19.80	2.8	ng	57145	6	20.00	415373	20.0