

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG122217\
 Data File : BG031728.D
 Acq On : 23 Dec 2017 1:40
 Operator : SJ/JU
 Sample : I7004-07
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 C-MW-11-121817

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_G\METHODS\8270-BG122117.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	3.447	19	27	38	rBV	88875	189150	3.98%	1.000%
2	3.541	38	43	49	rVB	30700	48378	1.02%	0.256%
3	6.238	495	502	513	rBV	309047	534521	11.26%	2.826%
4	7.918	779	788	799	rBB	195233	366136	7.71%	1.936%
5	8.336	850	859	869	rBV	607923	1111062	23.41%	5.874%
6	8.823	935	942	952	rBB	150462	271211	5.71%	1.434%
7	9.164	991	1000	1013	rVB	610690	1143433	24.09%	6.045%
8	10.022	1138	1146	1158	rBV	424070	802837	16.91%	4.244%
9	11.714	1423	1434	1444	rBV	210152	400860	8.44%	2.119%
10	14.088	1830	1838	1849	rVB	1718735	2756068	58.06%	14.570%
11	15.457	2064	2071	2080	rVB2	393845	655059	13.80%	3.463%
12	16.931	2315	2322	2333	rBV	1457488	2312861	48.72%	12.227%
13	18.195	2527	2537	2549	rBV	570560	904657	19.06%	4.782%
14	19.011	2671	2676	2686	rBV2	86012	127891	2.69%	0.676%
15	20.245	2882	2886	2896	rBV2	102701	157318	3.31%	0.832%
16	20.727	2961	2968	2976	rBV	3390975	4747035	100.00%	25.095%
17	22.096	3195	3201	3209	rBV2	68886	117154	2.47%	0.619%
18	22.548	3270	3278	3290	rVB2	598898	1122581	23.65%	5.934%
19	26.332	3909	3922	3934	rBV	344449	1148017	24.18%	6.069%

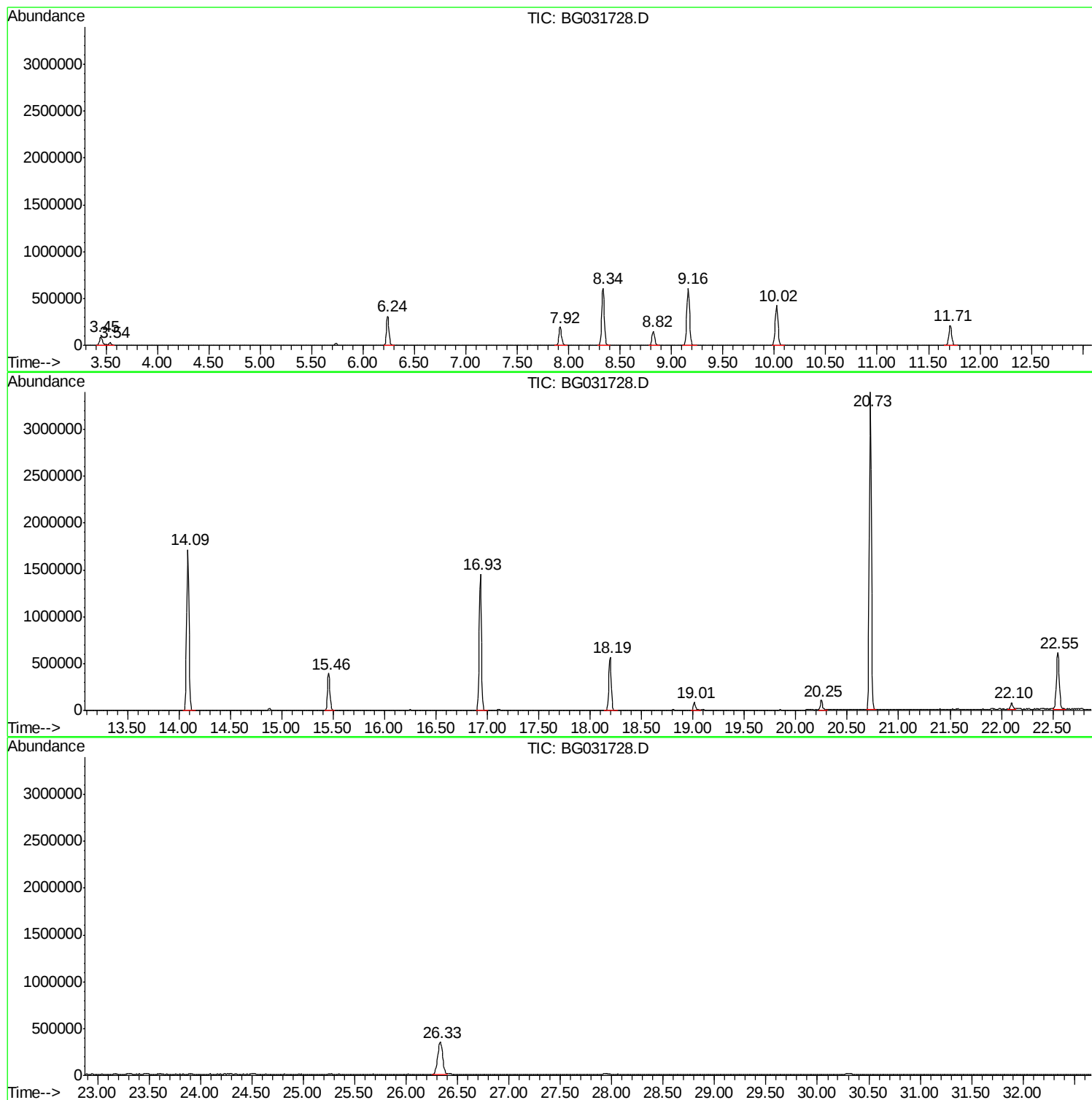
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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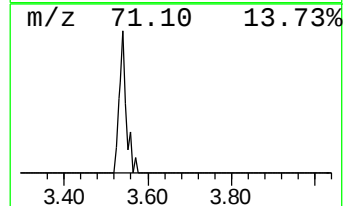
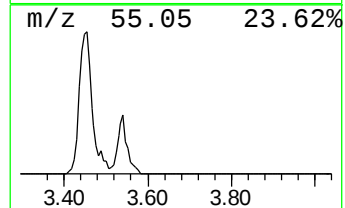
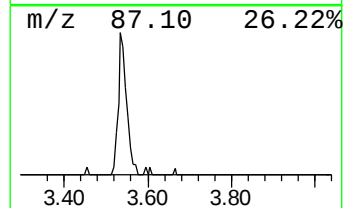
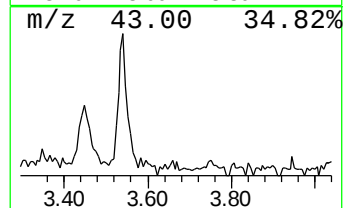
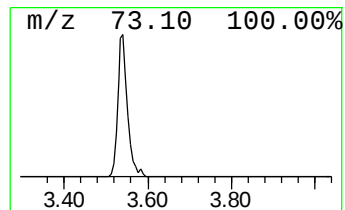
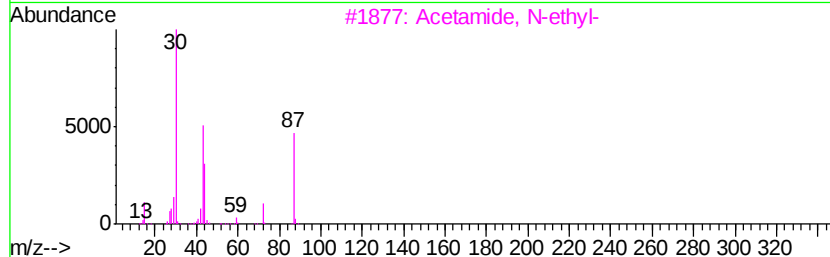
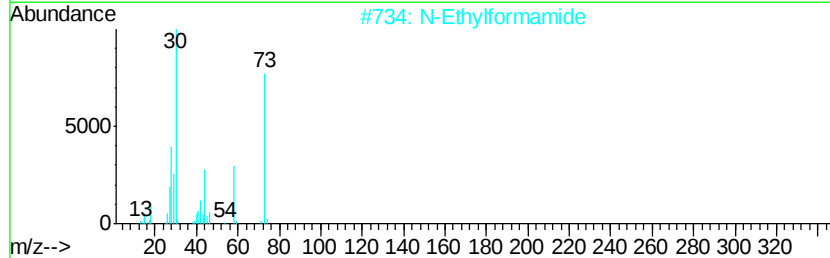
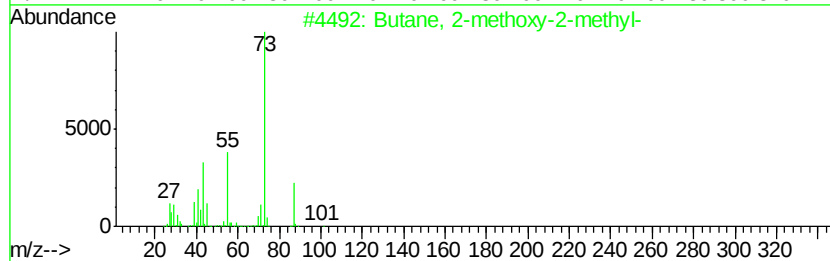
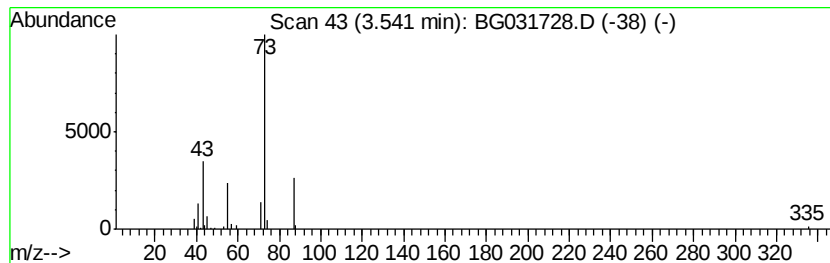
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Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.54	3.57 ng	48378	1,4-Dichlorobenzene-d4	8.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2		N-Ethylformamide	73	C3H7NO	000627-45-2	9
3		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9



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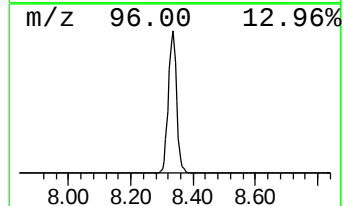
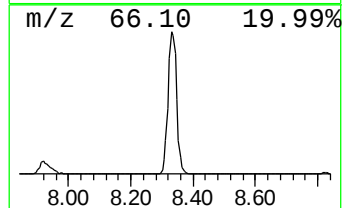
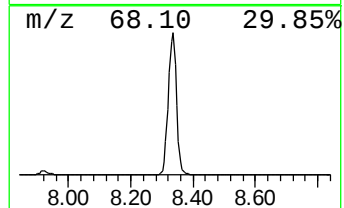
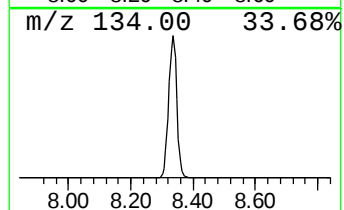
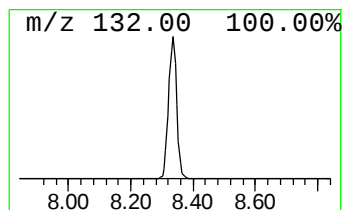
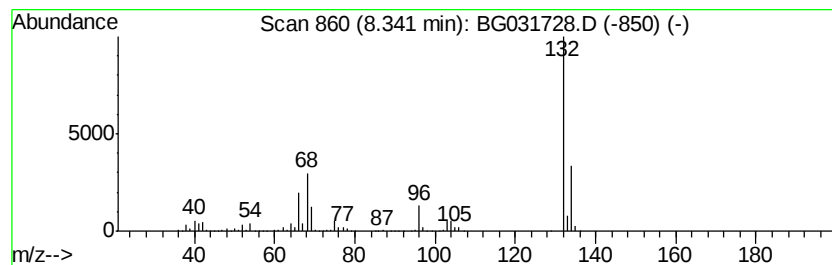
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown8.34 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.34	81.93 ng	1111060	1,4-Dichlorobenzene-d4	8.82

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	33
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	32
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	25
5		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	25



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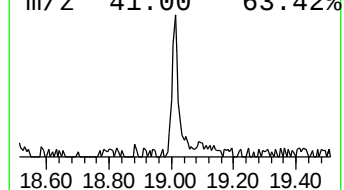
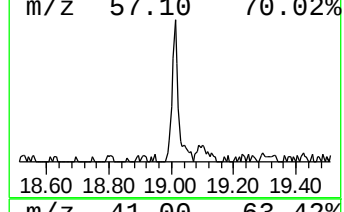
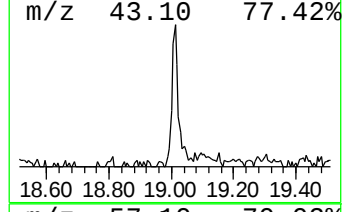
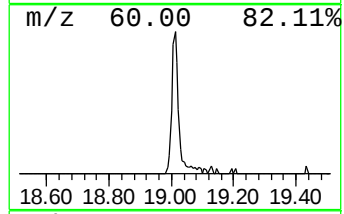
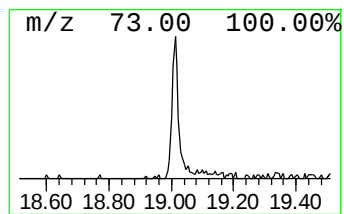
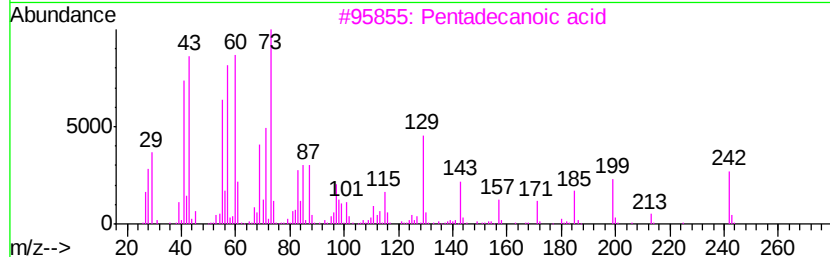
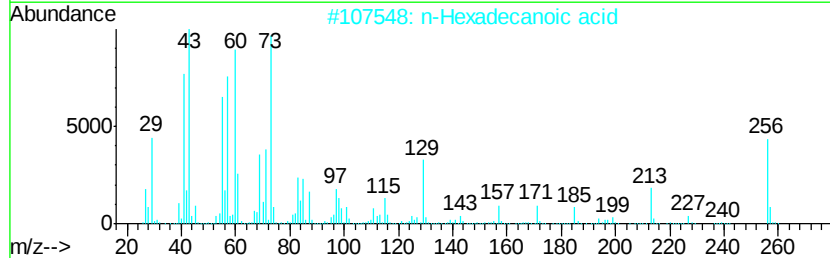
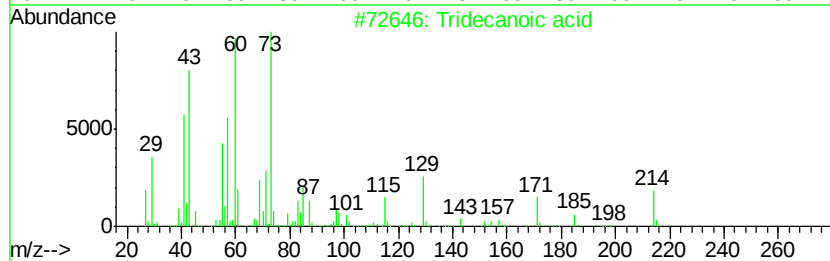
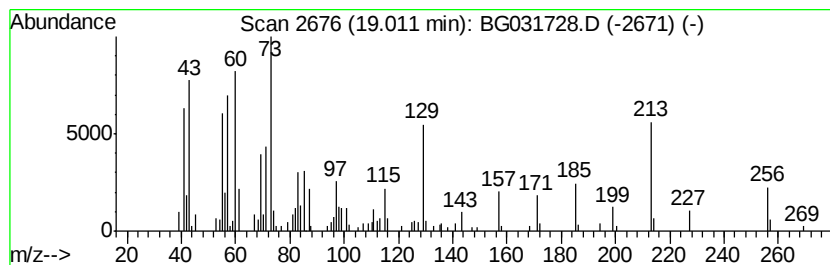
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Peak Number 5 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.01	2.83 ng	127891	Phenanthrene-d10	18.19

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	92
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4		n-Decanoic acid	172	C10H20O2	000334-48-5	55
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	52



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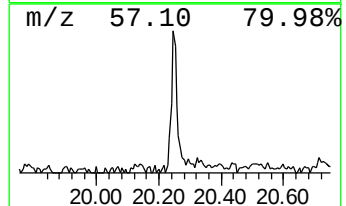
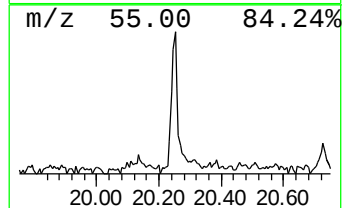
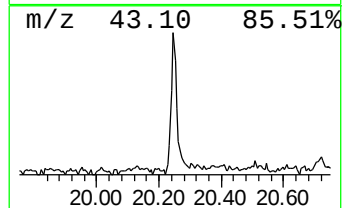
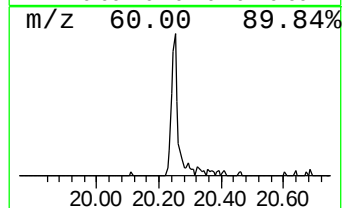
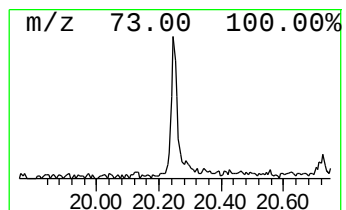
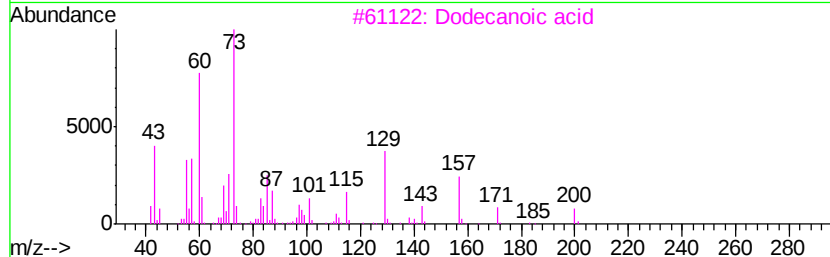
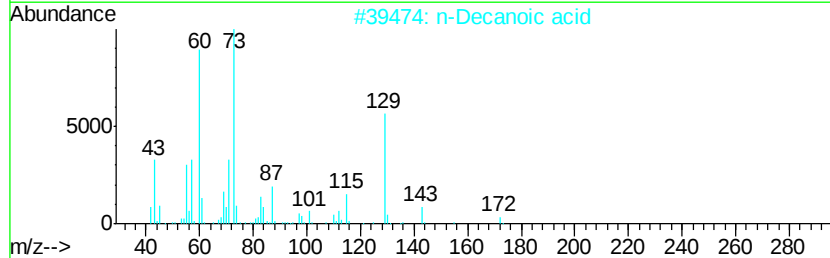
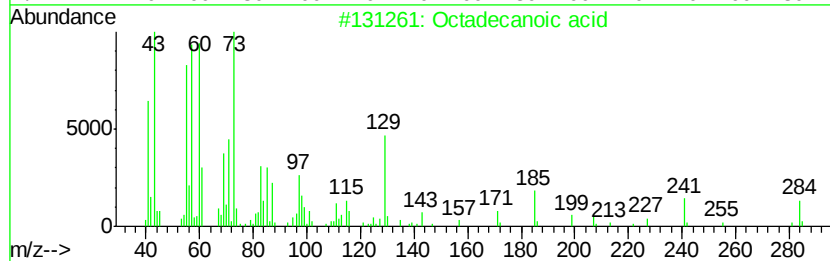
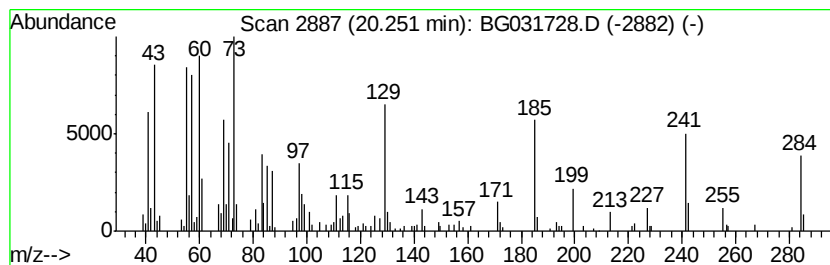
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Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.25	3.48 ng	157318	Phenanthrene-d10	18.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Decanoic acid	172	C10H20O2	000334-48-5	46
3	Dodecanoic acid	200	C12H24O2	000143-07-7	43
4	Tridecanoic acid	214	C13H26O2	000638-53-9	38
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	38



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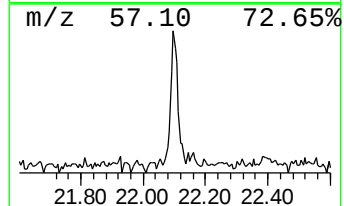
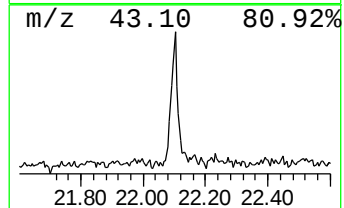
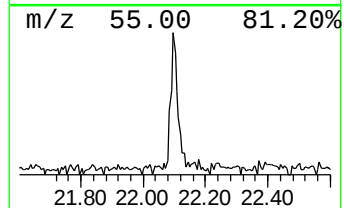
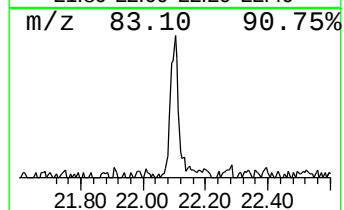
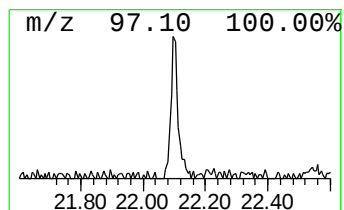
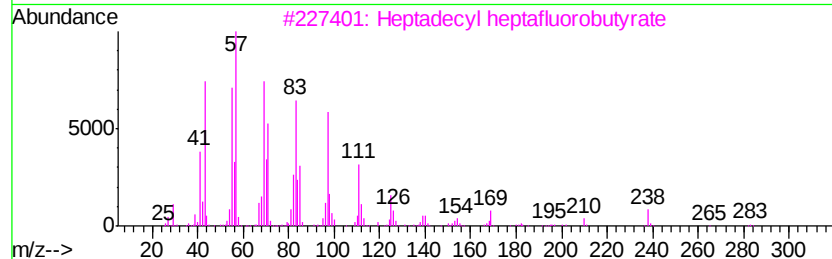
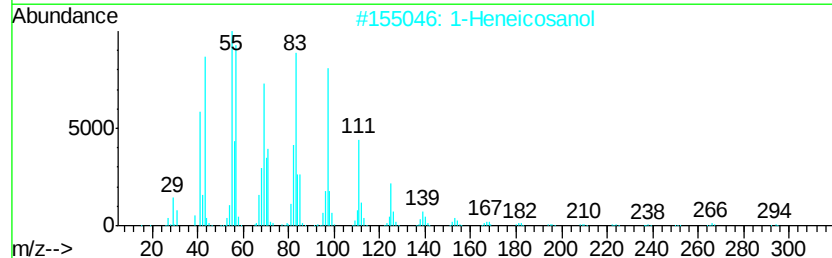
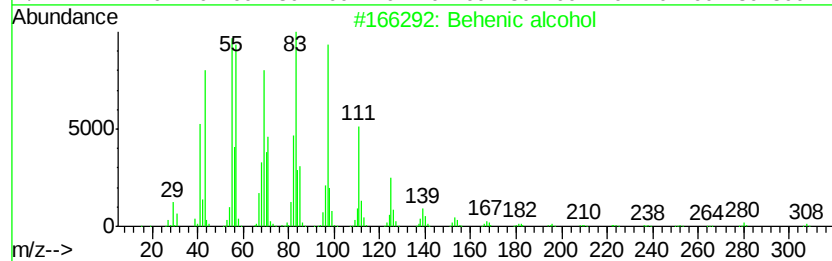
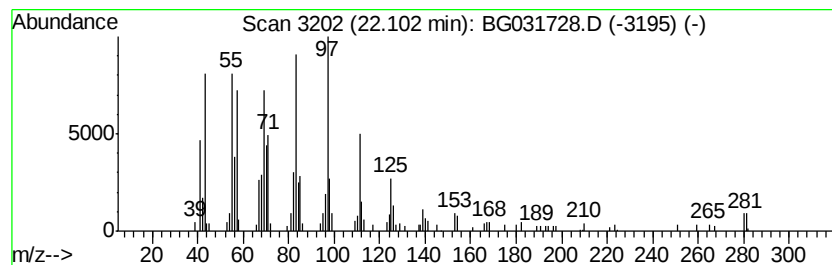
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Peak Number 7 Behenic alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.10	2.09 ng	117154	Chrysene-d12	22.55	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	81
2	1-Heneicosanol	312	C21H44O	015594-90-8	70
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	70
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	62
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	62



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.54	3.6	ng	48378	1	8.82	271211	20.0
unknown8.34	8.34	81.9	ng	1111060	1	8.82	271211	20.0
Tridecanoic acid	19.01	2.8	ng	127891	4	18.19	904657	20.0
Octadecanoic acid	20.25	3.5	ng	157318	4	18.19	904657	20.0
Behenic alcohol	22.10	2.1	ng	117154	5	22.55	1122580	20.0