

Data Path : Z:\HPCHEM1\BNA G\DATA\BG040518\
 Data File : BG033618.D
 Acq On : 6 Apr 2018 7:29
 Operator : SJ/JU
 Sample : J2224-03
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 040218-JETW-E-U-M

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-BG031918.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	3.476	27	32	43	rBV	126507	245154	5.88%	1.471%
2	3.564	43	47	56	rVB	108858	168591	4.05%	1.011%
3	6.284	505	510	526	rBV	143928	337119	8.09%	2.022%
4	7.976	792	798	816	rBV	84234	271725	6.52%	1.630%
5	8.370	858	865	884	rBV	349769	783219	18.80%	4.699%
6	8.858	942	948	958	rBV2	91292	217878	5.23%	1.307%
7	9.193	997	1005	1021	rBV	518443	1054834	25.32%	6.328%
8	10.062	1145	1153	1177	rBV	417377	1020381	24.49%	6.121%
9	11.743	1431	1439	1458	rBV	164732	370419	8.89%	2.222%
10	14.105	1834	1841	1859	rBV	1592151	2662790	63.92%	15.974%
11	14.898	1969	1976	1981	rBV2	101738	170283	4.09%	1.022%
12	15.303	2038	2045	2052	rBV2	46539	67069	1.61%	0.402%
13	15.479	2069	2075	2085	rBV2	353744	625215	15.01%	3.751%
14	16.243	2201	2205	2209	rVB	64653	79835	1.92%	0.479%
15	16.948	2319	2325	2337	rBV	860423	1486961	35.69%	8.920%
16	17.095	2345	2350	2362	rVB	57863	98808	2.37%	0.593%
17	17.882	2479	2484	2490	rBV2	35881	49857	1.20%	0.299%
18	18.206	2529	2539	2552	rBV2	501945	872366	20.94%	5.233%
19	19.005	2671	2675	2681	rBV3	40631	65475	1.57%	0.393%
20	20.726	2962	2968	2988	rBV	2949662	4165987	100.00%	24.992%
21	22.066	3191	3196	3204	rBV2	47236	90765	2.18%	0.545%
22	22.553	3271	3279	3292	rBV	462931	955265	22.93%	5.731%
23	26.314	3908	3919	3938	rBV3	224776	809370	19.43%	4.855%

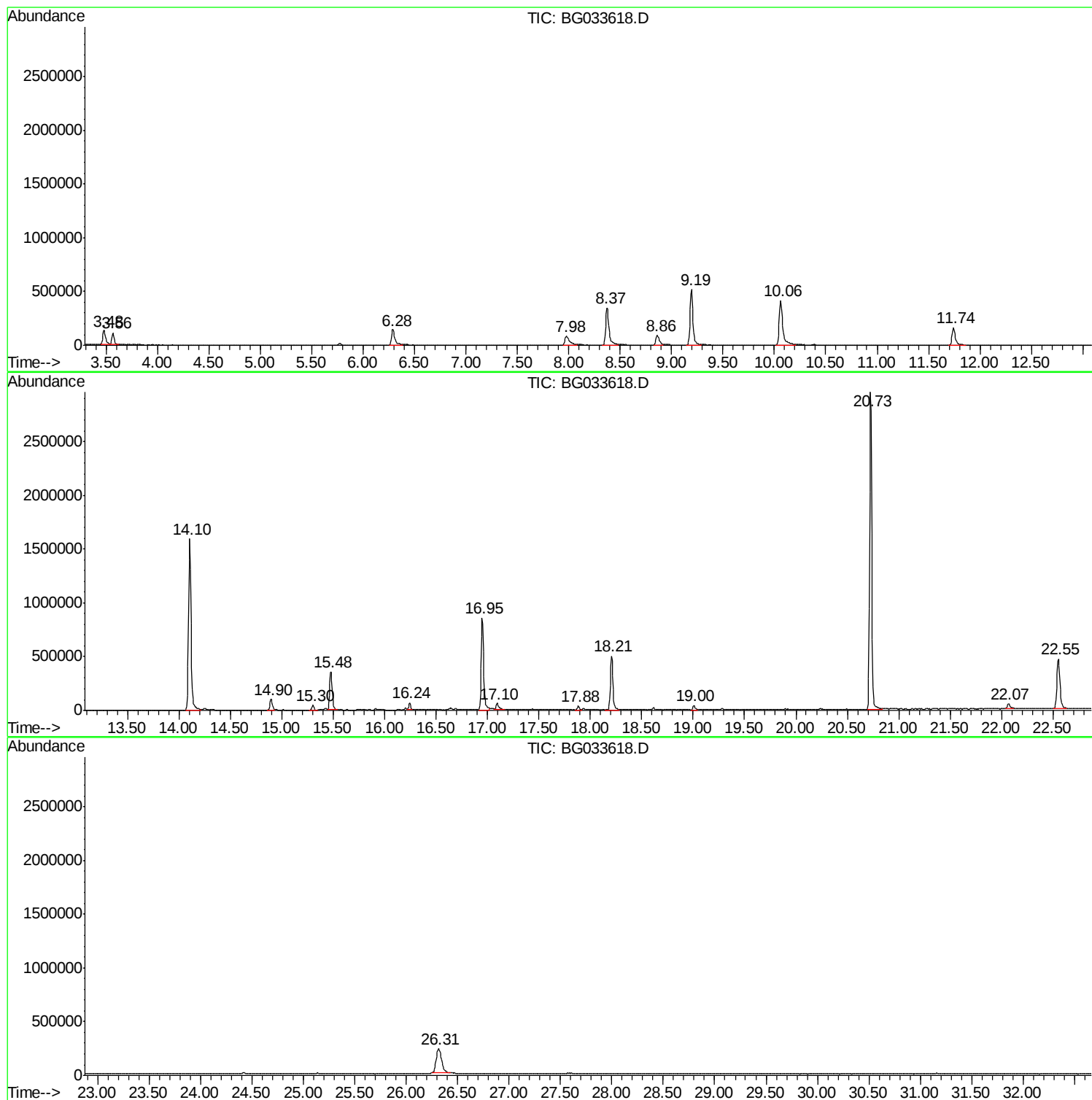
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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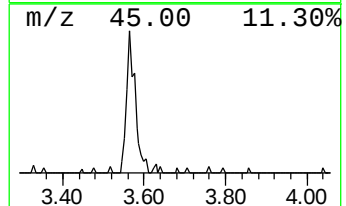
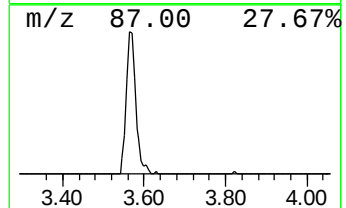
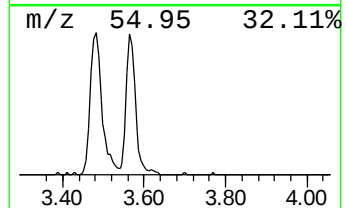
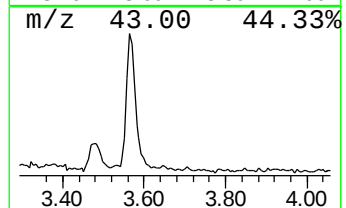
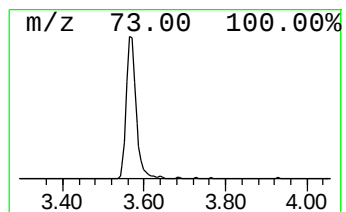
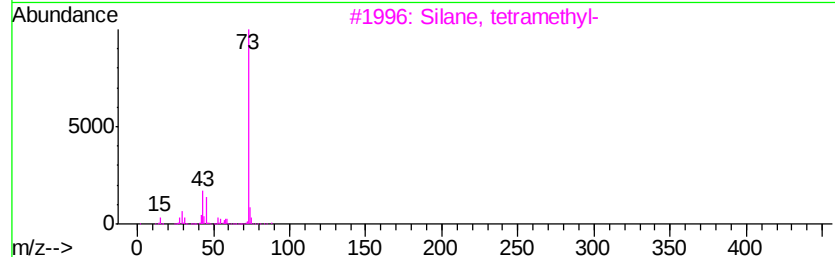
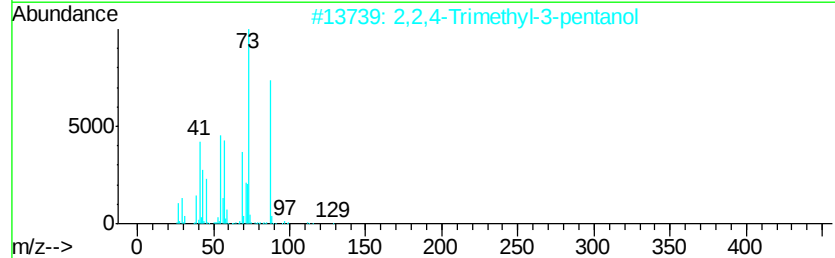
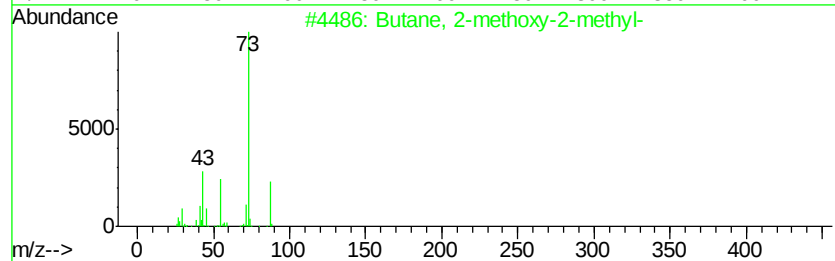
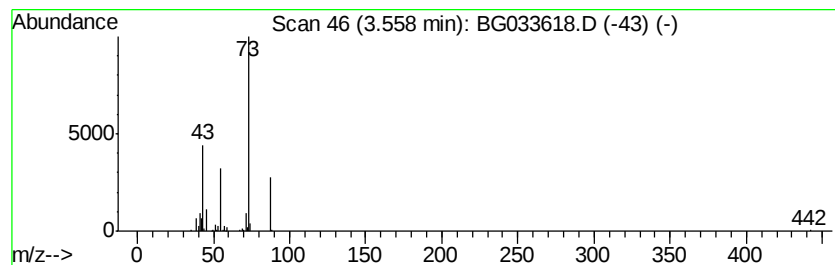
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.56	15.48 ng	168591	1,4-Dichlorobenzene-d4	8.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4		2,5-Dimethyl-4-hydroxy-3-hexanone	144	C8H16O2	000815-77-0	33
5		Butanoic acid, 2-hydroxy-2-methyl-	132	C6H12O3	032793-34-3	32



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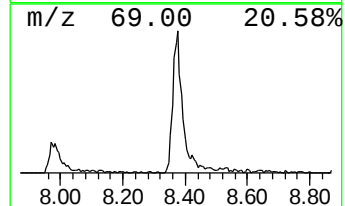
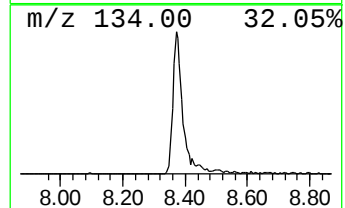
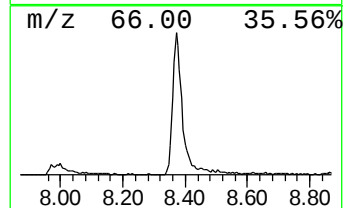
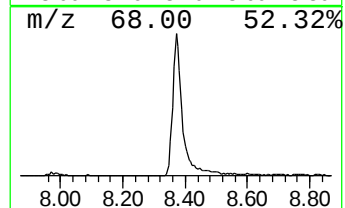
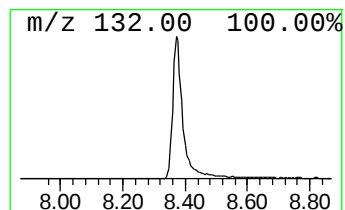
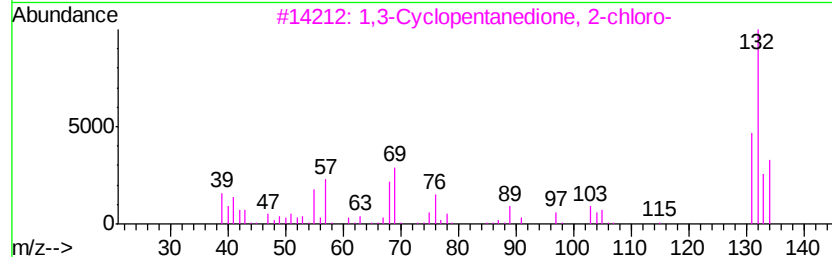
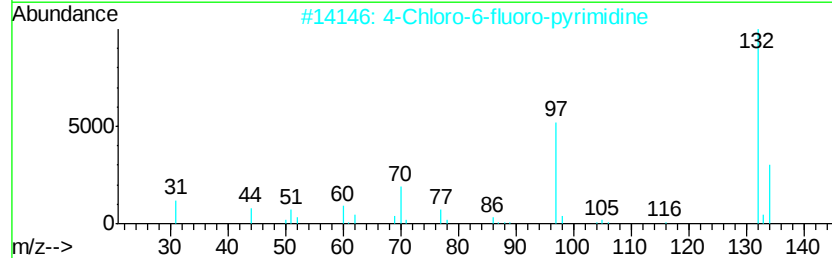
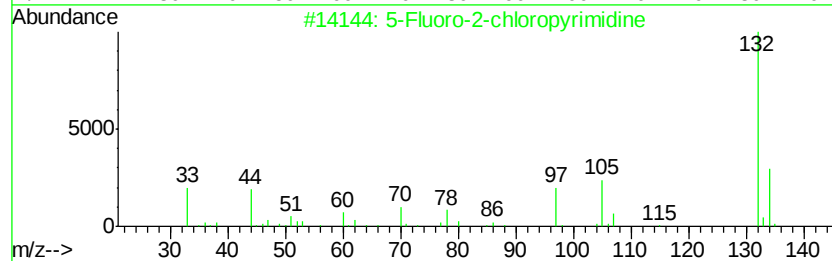
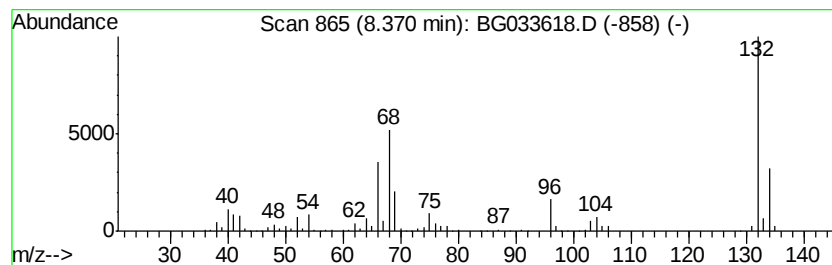
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown8.37 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.37	71.90 ng	783219	1,4-Dichlorobenzene-d4	8.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	23
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
5		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16



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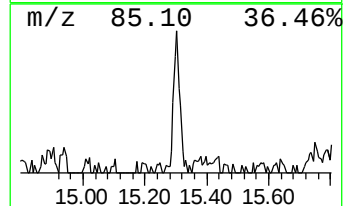
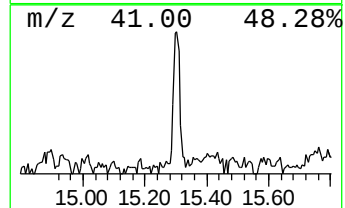
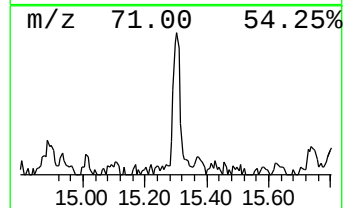
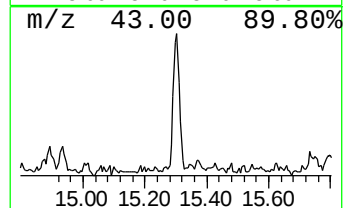
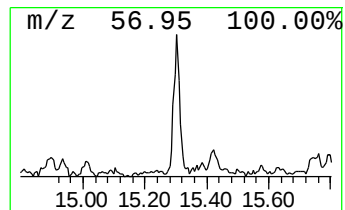
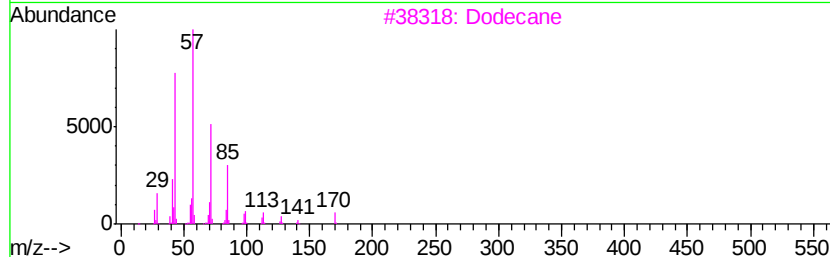
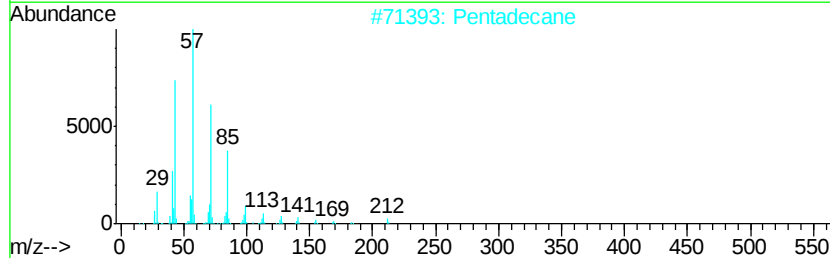
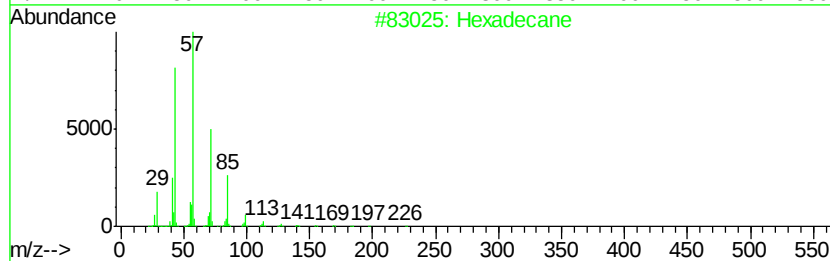
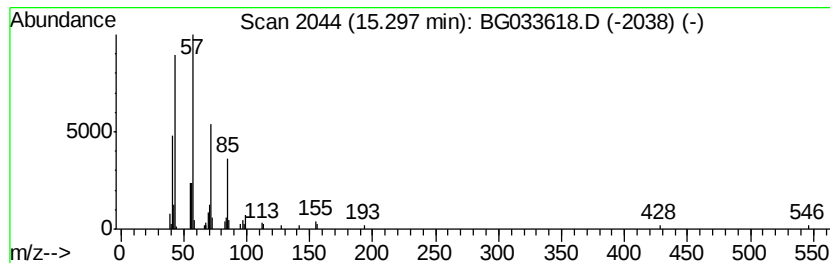
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Peak Number 5 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.30	2.15 ng	67069	Acenaphthene-d10	15.47

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	90
2	Pentadecane		212	C15H32	000629-62-9	83
3	Dodecane		170	C12H26	000112-40-3	78
4	Eicosane		282	C20H42	000112-95-8	78
5	Tetratetracontane		619	C44H90	007098-22-8	78



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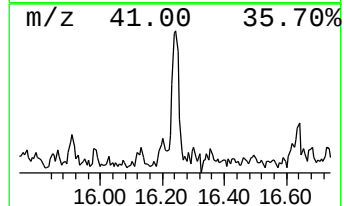
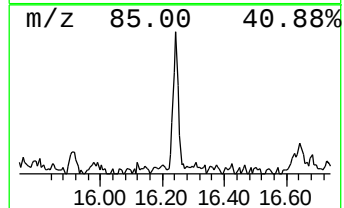
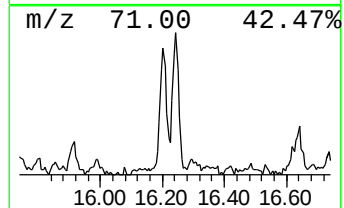
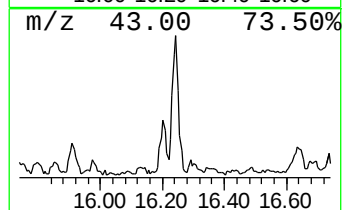
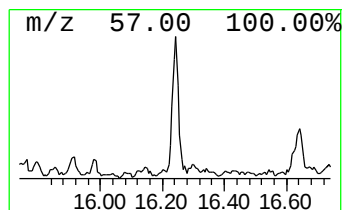
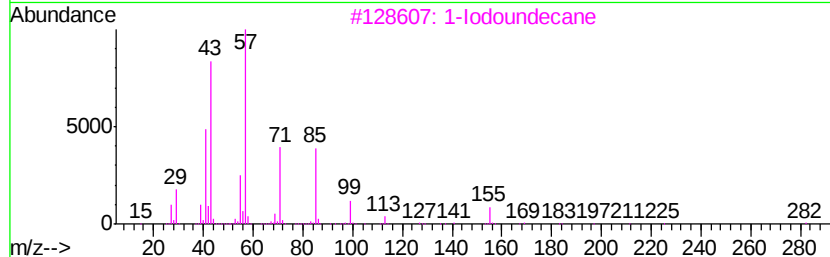
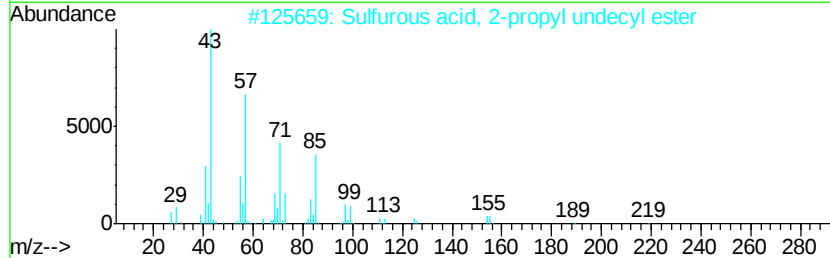
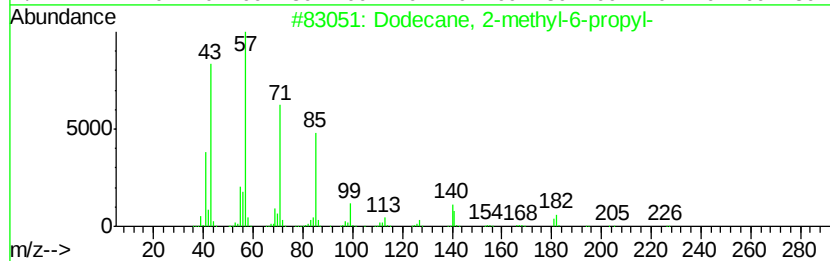
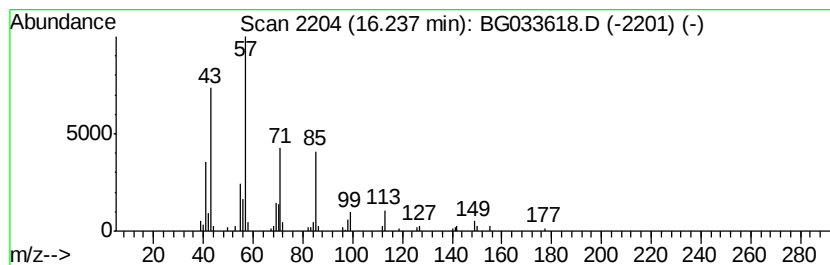
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Peak Number 6 Dodecane, 2-methyl-6-propyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.24	2.55 ng	79835	Acenaphthene-d10	15.47	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	90
2	Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	72
3	1-Iodoundecane	282	C11H23I	004282-44-4	72
4	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	72
5	Tetradecane	198	C14H30	000629-59-4	72



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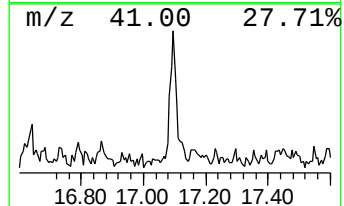
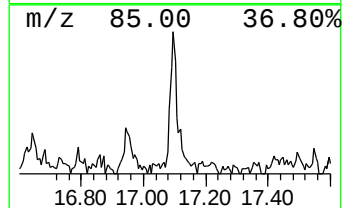
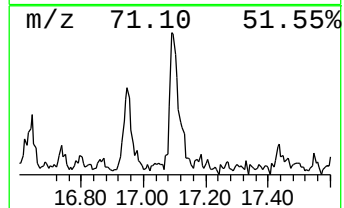
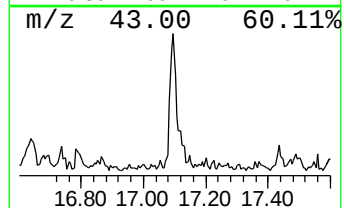
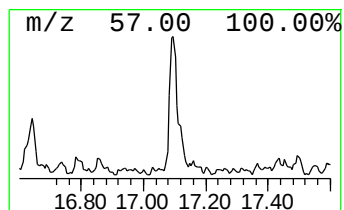
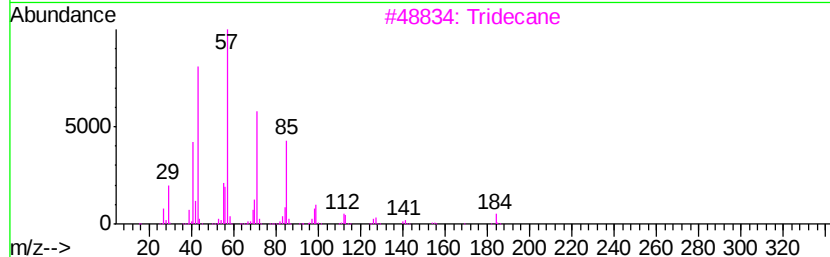
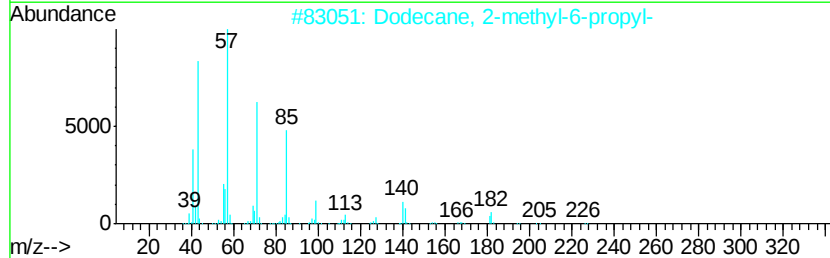
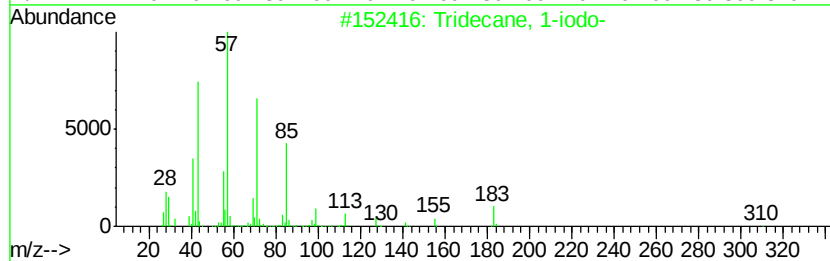
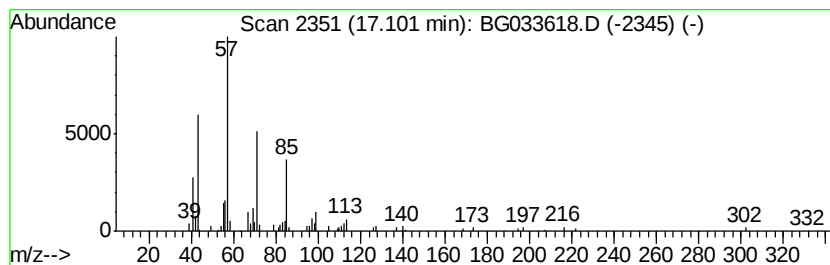
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Peak Number 7 Tridecane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.10	2.27 ng	98808	Phenanthrene-d10	18.21

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80
2		Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	78
3		Tridecane	184	C13H28	000629-50-5	78
4		Tetradecane	198	C14H30	000629-59-4	78
5		Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.56	15.5	ng	168591	1	8.86	217878	20.0
unknown8.37	8.37	71.9	ng	783219	1	8.86	217878	20.0
Hexadecane	15.30	2.1	ng	67069	3	15.47	625215	20.0
Dodecane, 2-methy...	16.24	2.5	ng	79835	3	15.47	625215	20.0
Tridecane, 1-iodo-	17.10	2.3	ng	98808	4	18.21	872366	20.0