

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061516\
 Data File : BF088066.D
 Acq On : 16 Jun 2016 6:53
 Operator : UM/SJ
 Sample : H3570-16
 Misc :
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-18-COMP

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_F\METHODS\8270-BF060716.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	1.701	7	10	18	rVB	166236	383446	13.86%	1.944%
2	1.815	18	20	31	rVV	1538299	2766265	100.00%	14.023%
3	1.953	31	32	70	rVB	97256	473563	17.12%	2.401%
4	4.901	288	290	300	rVB	81197	111000	4.01%	0.563%
5	5.336	325	328	330	rBV	1419440	1664025	60.15%	8.435%
6	6.376	417	419	422	rBV	1161173	1654672	59.82%	8.388%
7	6.513	428	431	433	rBV	1255986	1705896	61.67%	8.648%
8	6.742	448	451	453	rBV	675376	576597	20.84%	2.923%
9	6.902	462	465	467	rBV	1106511	1365819	49.37%	6.924%
10	7.313	498	501	503	rBV	879275	1099214	39.74%	5.572%
11	8.033	561	564	566	rBV	557376	733599	26.52%	3.719%
12	9.108	655	658	660	rBV	2028308	1744307	63.06%	8.842%
13	9.508	690	693	695	rBV	426216	414498	14.98%	2.101%
14	9.782	714	717	719	rVV	899635	806085	29.14%	4.086%
15	10.216	754	755	757	rVB	50843	46380	1.68%	0.235%
16	10.433	771	774	778	rBV	16656	34865	1.26%	0.177%
17	10.571	783	786	788	rBV2	676342	923572	33.39%	4.682%
18	10.696	795	797	801	rBV	47325	79276	2.87%	0.402%
19	11.142	834	836	837	rBV	26036	28928	1.05%	0.147%
20	11.256	844	846	849	rBV	757859	661837	23.93%	3.355%
21	12.845	982	985	987	rBV	1247872	1227594	44.38%	6.223%
22	13.748	1062	1064	1074	rBV	43053	97499	3.52%	0.494%
23	13.885	1074	1076	1079	rBV	482714	544402	19.68%	2.760%
24	14.651	1141	1143	1147	rBV2	17992	32993	1.19%	0.167%
25	15.291	1196	1199	1201	rBV	430277	550122	19.89%	2.789%

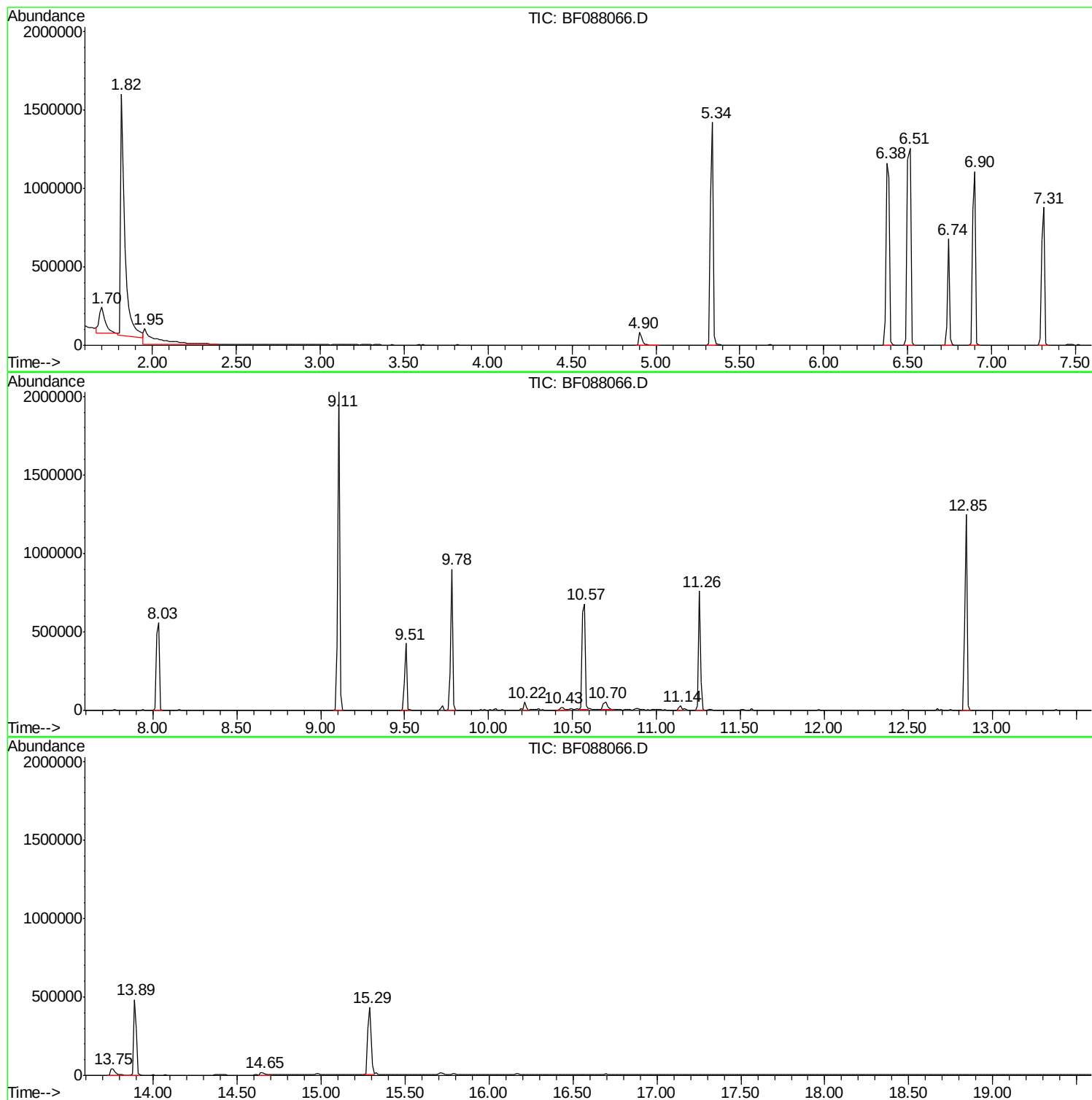
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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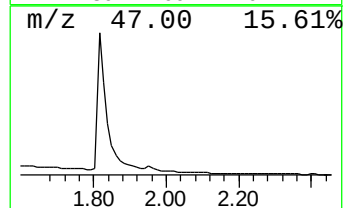
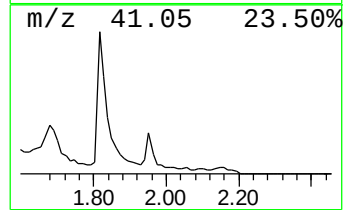
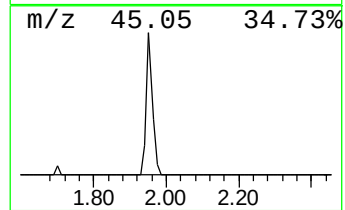
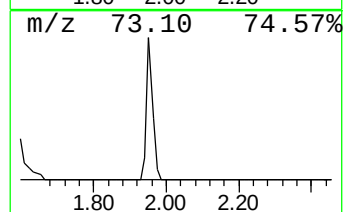
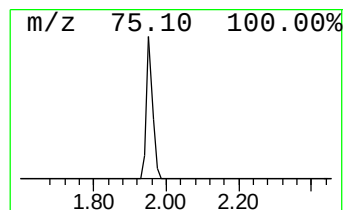
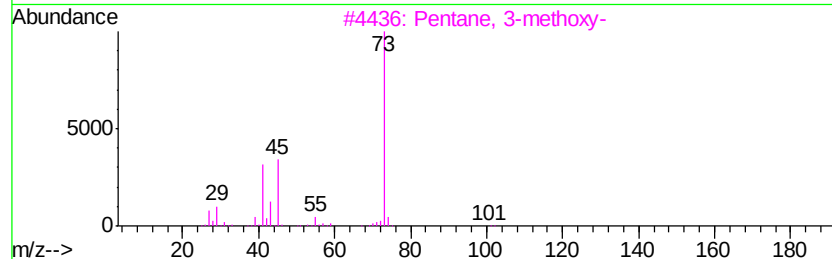
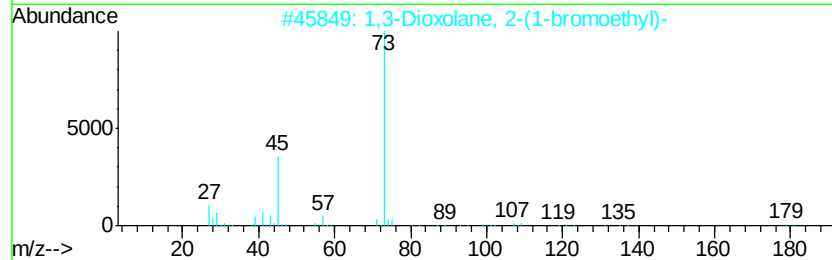
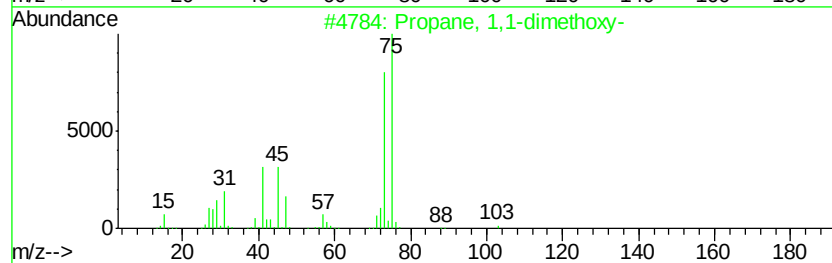
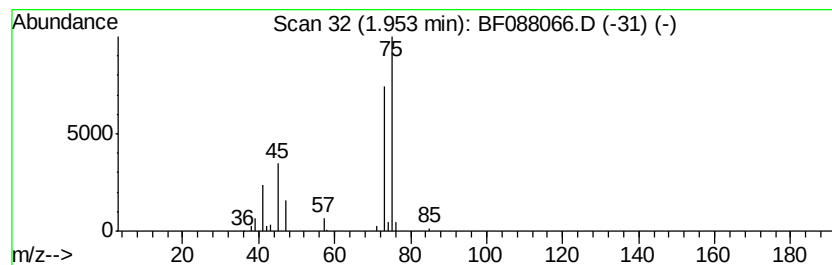
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.95	16.43 ng	473563	1,4-Dichlorobenzene-d4	6.74

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	10
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10
4		1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	9
5		Silanol, trimethyl-	90	C3H10OSi	001066-40-6	9



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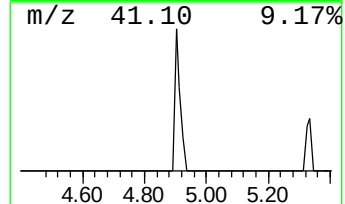
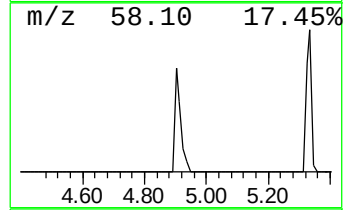
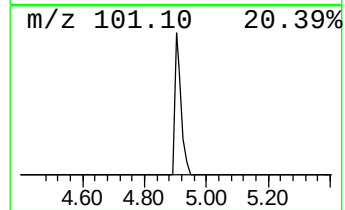
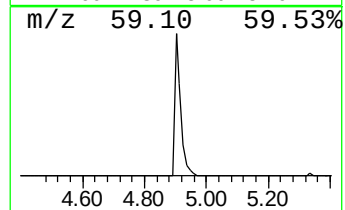
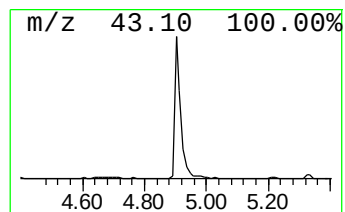
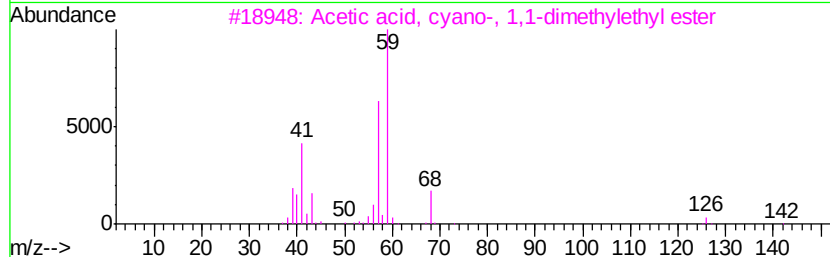
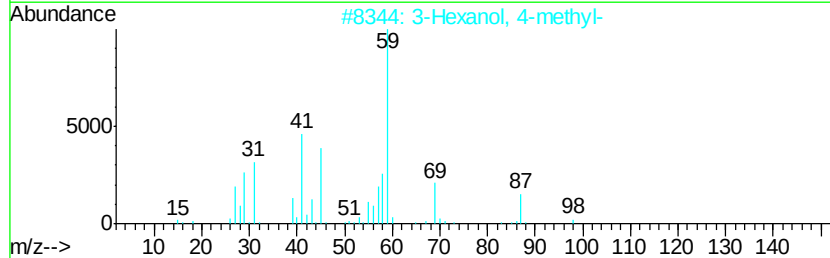
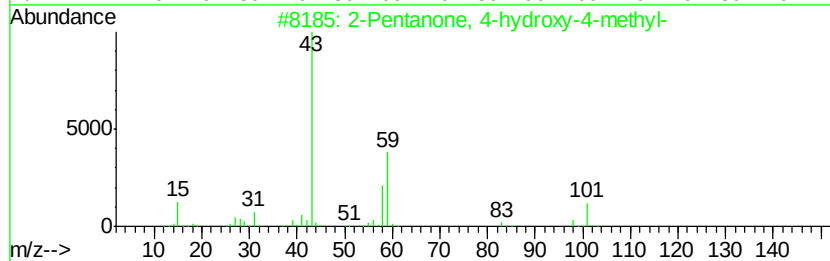
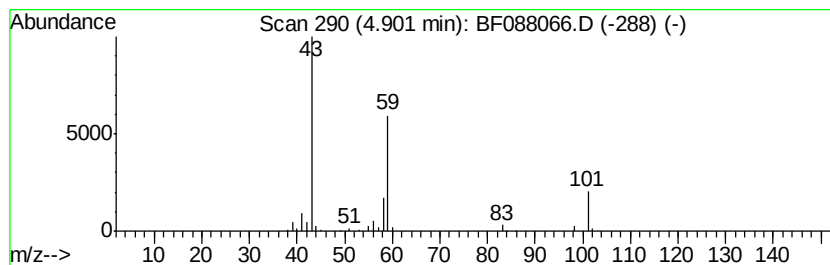
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TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	3.85 ng	111000	1,4-Dichlorobenzene-d4	6.74

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53	
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28	
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23	
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12	
5	Acetone	58	C3H6O	000067-64-1	9	



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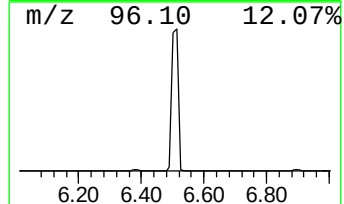
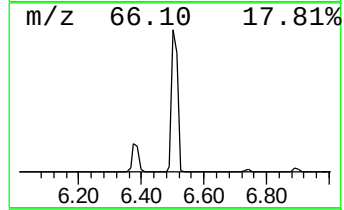
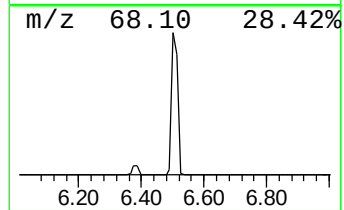
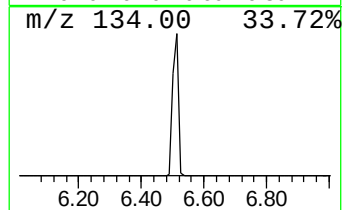
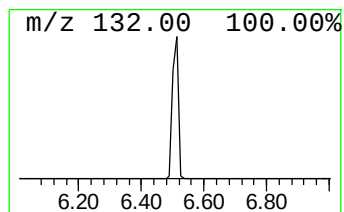
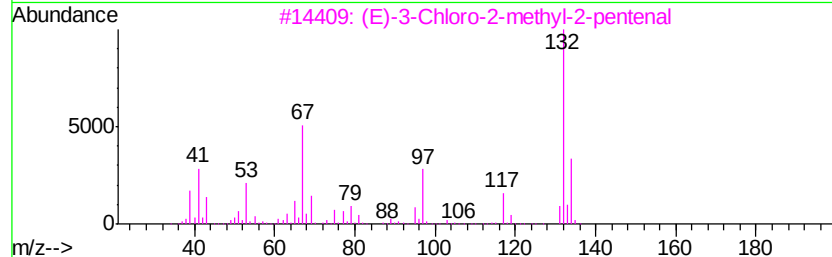
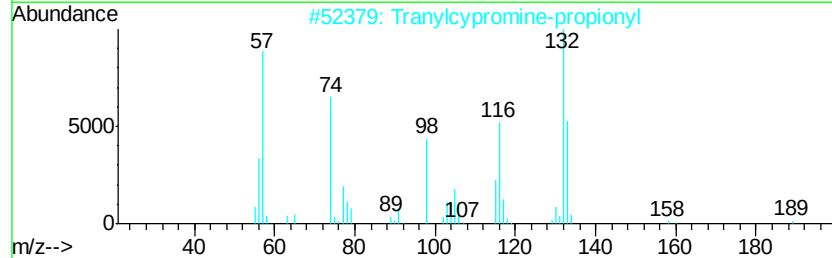
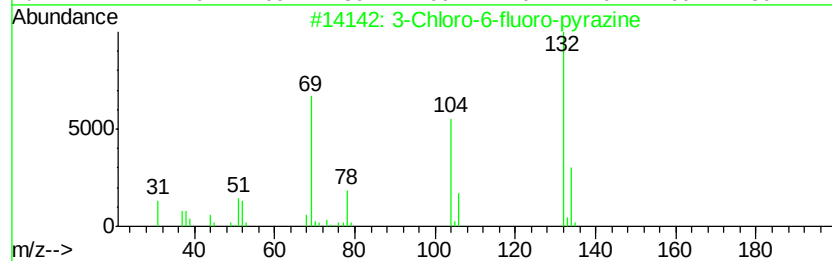
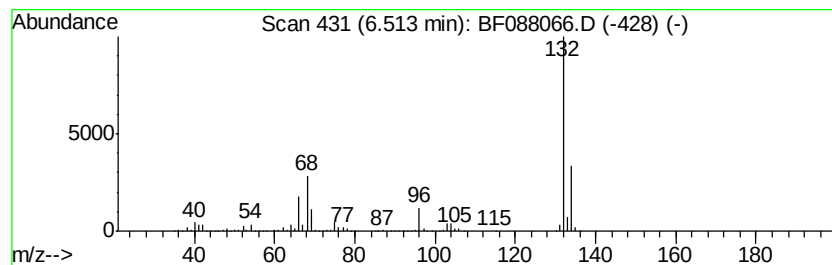
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Peak Number 5 3-Chloro-6-fluoro-pyrazine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	59.17 ng	1705900	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	50
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	37
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	33
4		Amphetaminil	250	C17H18N2	017590-01-1	28
5		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	25



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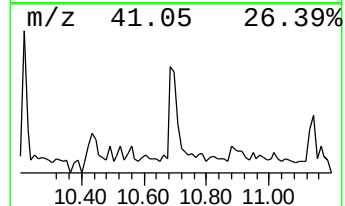
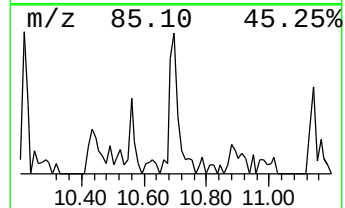
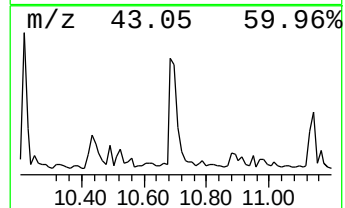
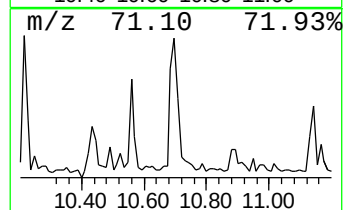
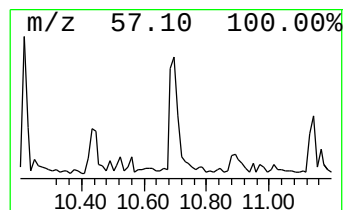
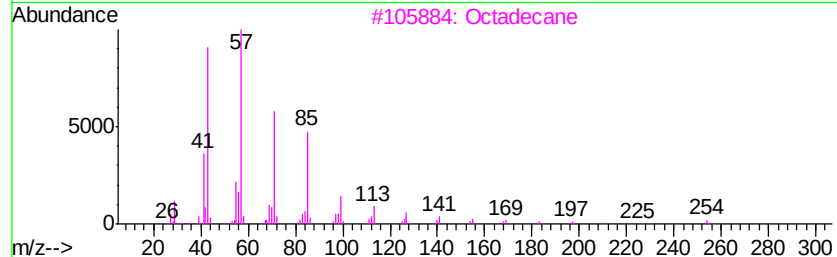
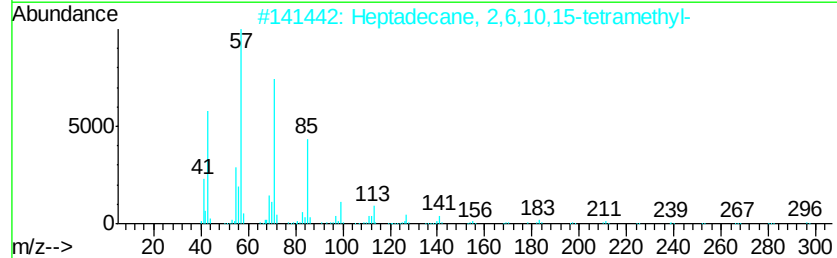
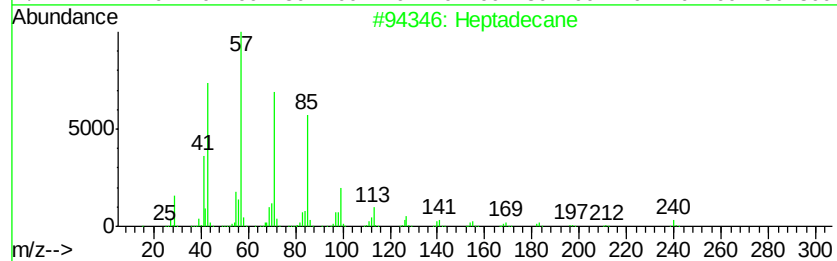
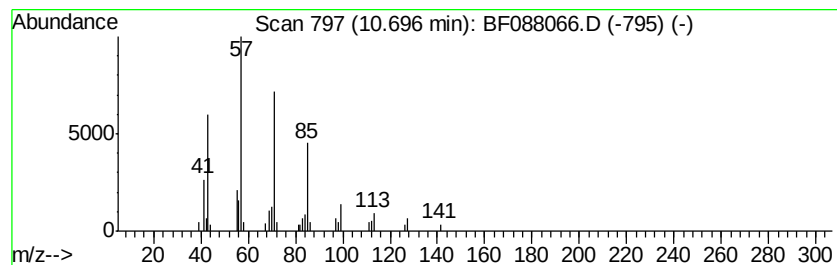
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Peak Number 7 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.70	2.40 ng	79276	Phenanthrene-d10	11.26	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
3	Octadecane	254	C18H38	000593-45-3	91
4	Hexadecane	226	C16H34	000544-76-3	90
5	Tetracosane	338	C24H50	000646-31-1	87



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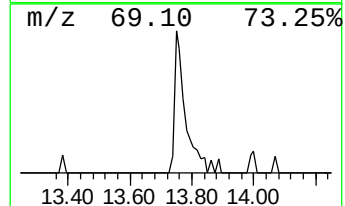
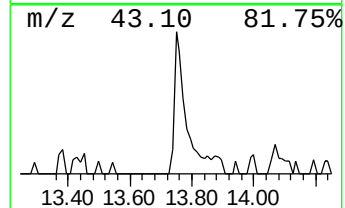
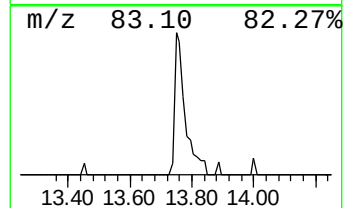
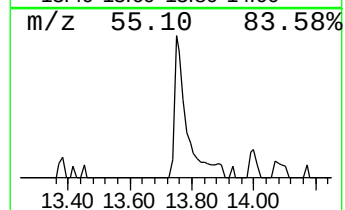
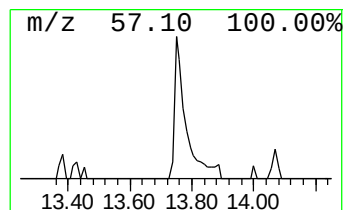
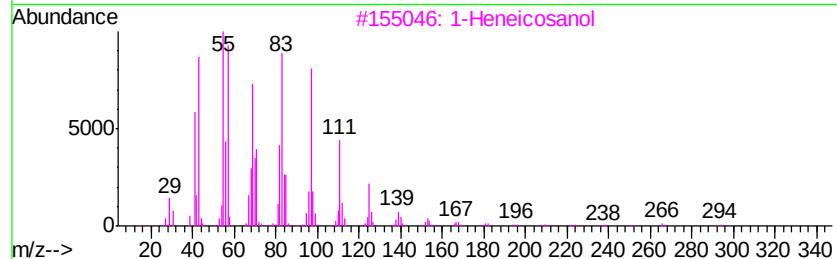
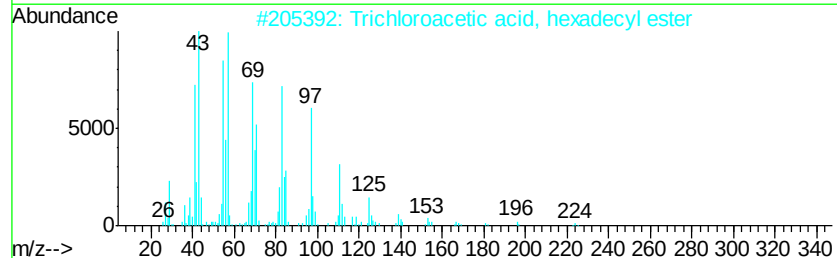
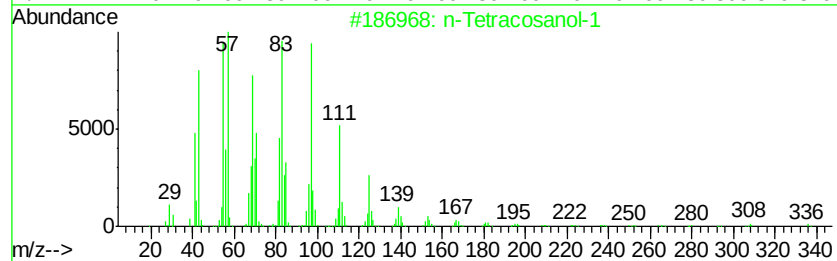
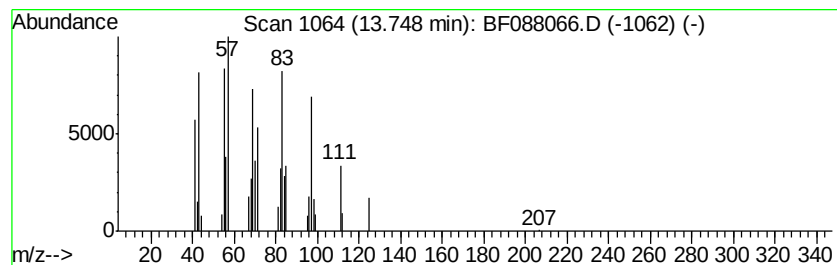
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Peak Number 8 n-Tetracosanol-1 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.75	3.58 ng	97499	Chrysene-d12	13.89	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	1-Heneicosanol	312	C21H44O	015594-90-8	91
4	1-Heptacosanol	396	C27H56O	002004-39-9	91
5	Trifluoroacetox y hexadecane	338	C18H33F3O2	006222-03-3	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-dime...	1.95	16.4	ng	473563	1	6.74	576597	20.0
2-Pentanone, 4-hy...	4.90	3.9	ng	111000	1	6.74	576597	20.0
3-Chloro-6-fluoro...	6.51	59.2	ng	1705900	1	6.74	576597	20.0
Heptadecane	10.70	2.4	ng	79276	4	11.26	661837	20.0
n-Tetracosanol-1	13.75	3.6	ng	97499	5	13.89	544402	20.0