

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080116\
 Data File : BF089509.D
 Acq On : 1 Aug 2016 14:06
 Operator : UM/SJ
 Sample : H4285-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 AB-SLOPE(0-4)K

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-BF072716.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	1.655	4	6	42	rVB	707163	1870222	100.00%	14.480%
2	4.570	258	261	273	rVB	214913	387216	20.70%	2.998%
3	5.050	301	303	326	rBV	935891	1213835	64.90%	9.398%
4	6.147	397	399	401	rBV	1136725	1272207	68.02%	9.850%
5	6.250	406	408	410	rBV	1308912	1353239	72.36%	10.477%
6	6.479	426	428	439	rVB	217939	234578	12.54%	1.816%
7	6.639	439	442	444	rBV	725678	970583	51.90%	7.515%
8	7.050	476	478	489	rBV	571881	796494	42.59%	6.167%
9	7.770	538	541	543	rBV	220361	303774	16.24%	2.352%
10	8.845	632	635	638	rBV	1378249	1327187	70.96%	10.275%
11	9.245	668	670	673	rBV	206294	177939	9.51%	1.378%
12	9.508	691	693	695	rBV	435504	384013	20.53%	2.973%
13	9.965	731	733	735	rVB	31444	24503	1.31%	0.190%
14	10.182	749	752	755	rBV	11053	19763	1.06%	0.153%
15	10.296	760	762	764	rBV	606490	653243	34.93%	5.058%
16	10.433	772	774	778	rBV	40006	41586	2.22%	0.322%
17	10.982	819	822	824	rBV	319079	344919	18.44%	2.670%
18	11.542	869	871	875	rBV	15414	21856	1.17%	0.169%
19	12.319	936	939	945	rBV	17578	25067	1.34%	0.194%
20	12.559	958	960	963	rBV	800311	926183	49.52%	7.171%
21	13.474	1038	1040	1045	rBV	40265	57882	3.09%	0.448%
22	13.599	1049	1051	1059	rBV	247218	254931	13.63%	1.974%
23	14.457	1123	1126	1128	rBV	60846	68308	3.65%	0.529%
24	14.925	1165	1167	1170	rBV	169077	186562	9.98%	1.444%

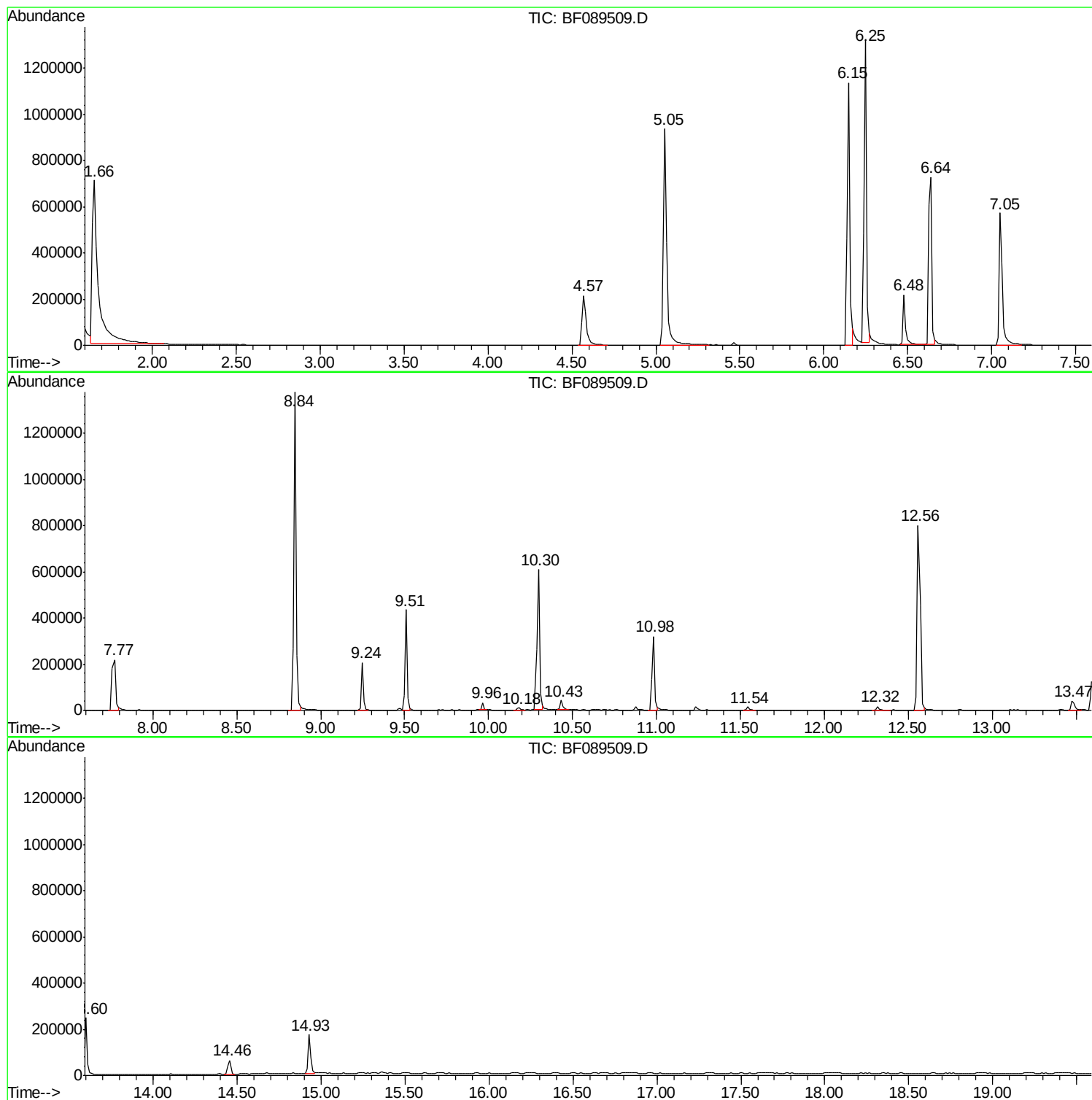
Sum of corrected areas: 12916090

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.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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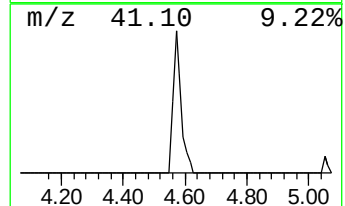
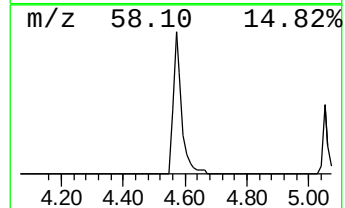
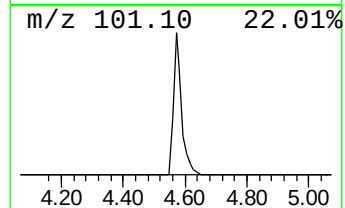
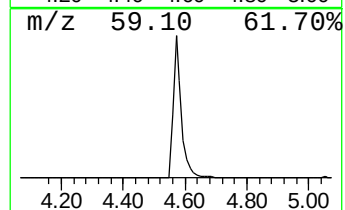
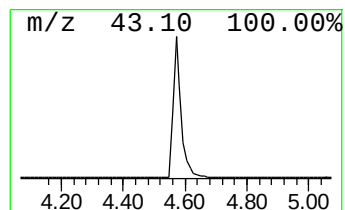
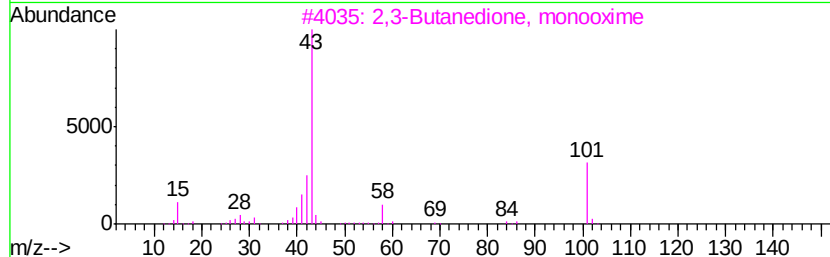
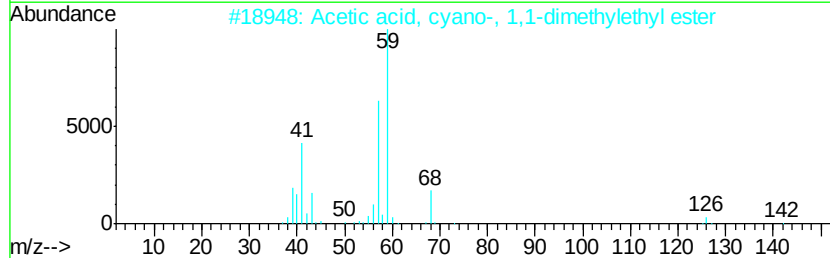
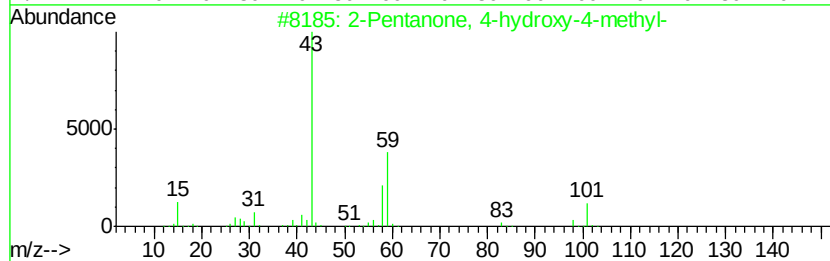
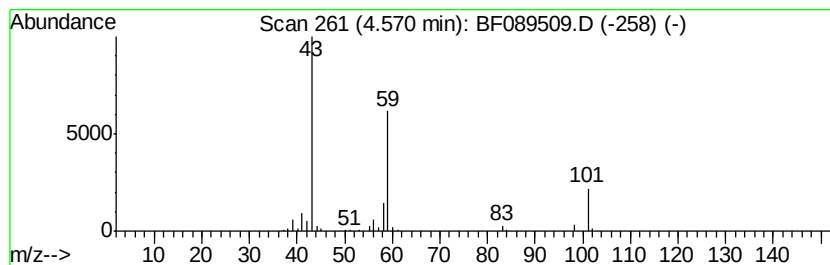
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.57	33.01 ng	387216	1,4-Dichlorobenzene-d4	6.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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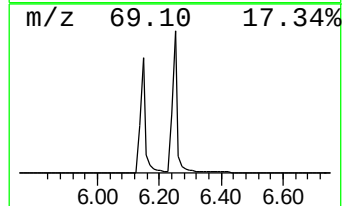
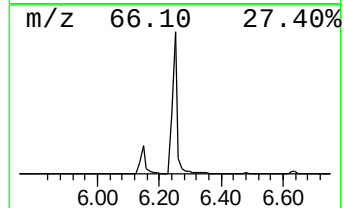
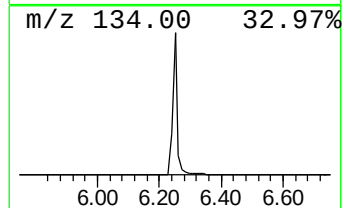
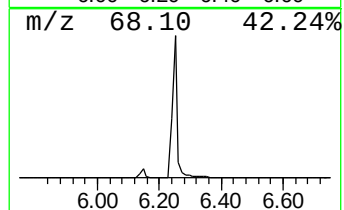
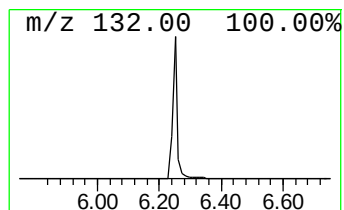
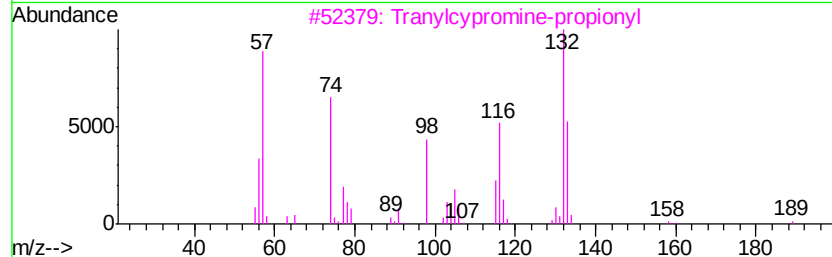
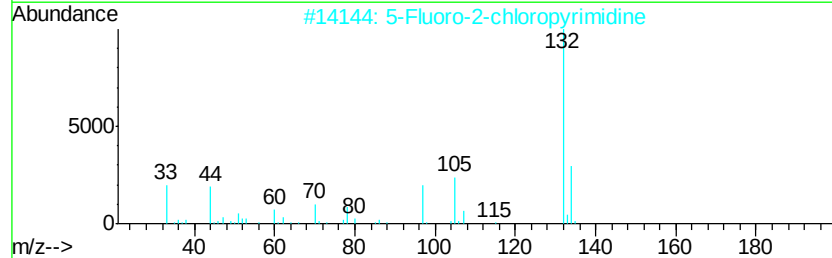
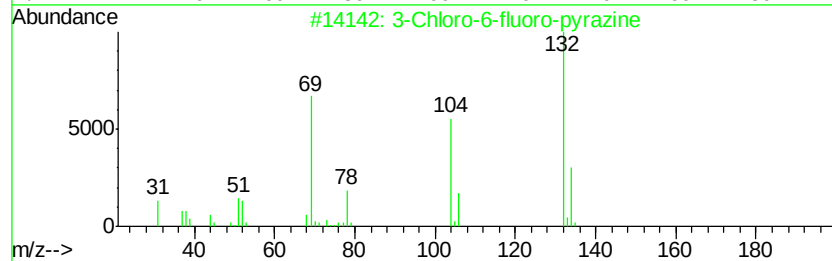
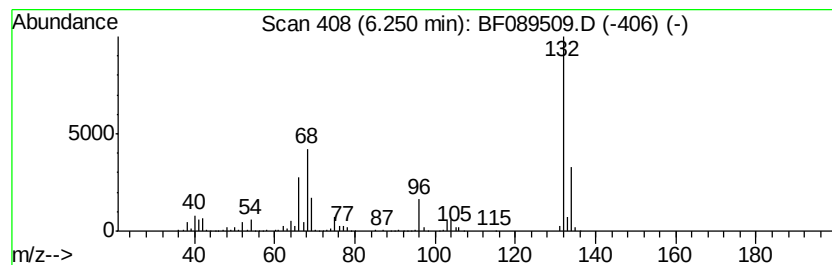
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Peak Number 3 unknown6.25 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.25	115.38 ng	1353240	1,4-Dichlorobenzene-d4	6.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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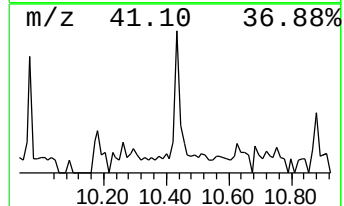
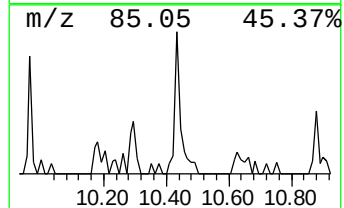
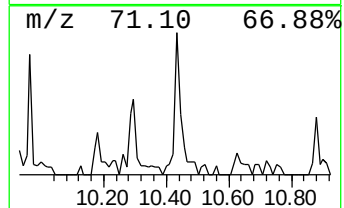
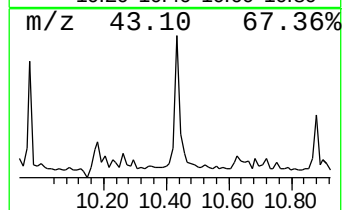
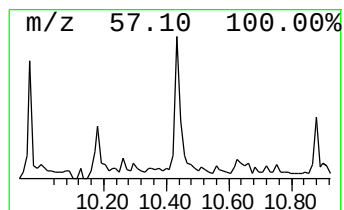
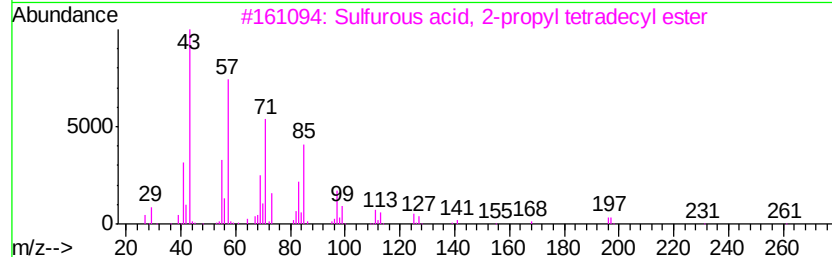
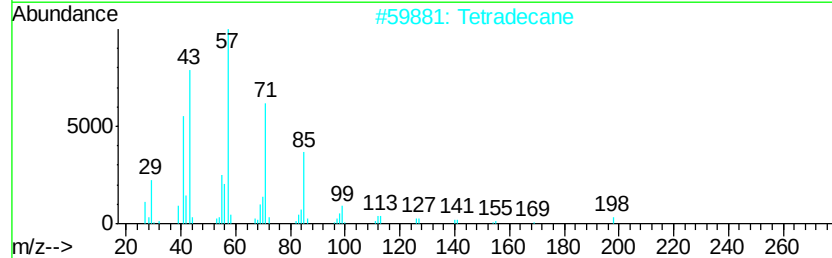
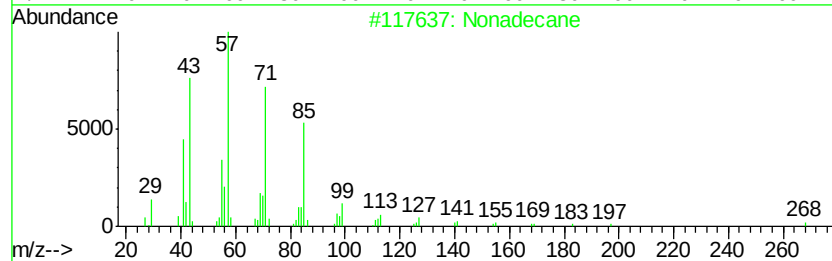
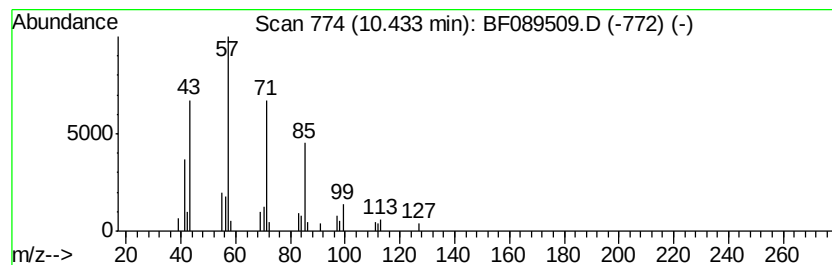
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Peak Number 5 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.43	2.41 ng	41586	Phenanthrene-d10		10.98
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	86
2	Tetradecane	198	C14H30	000629-59-4	86
3	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	86
4	Pentadecane	212	C15H32	000629-62-9	86
5	Hexadecane	226	C16H34	000544-76-3	83



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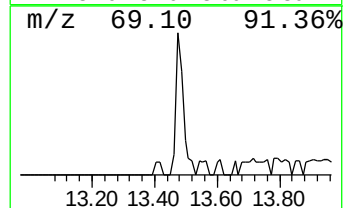
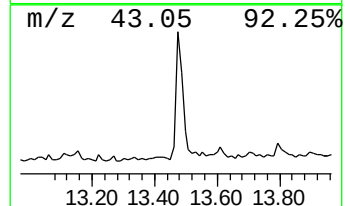
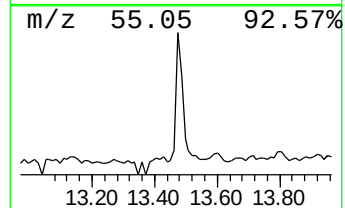
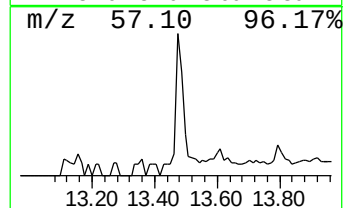
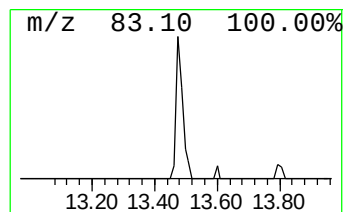
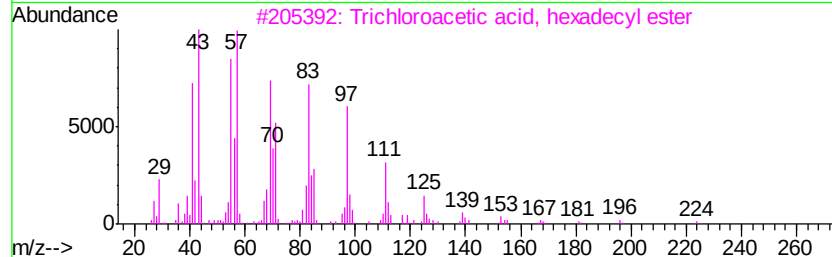
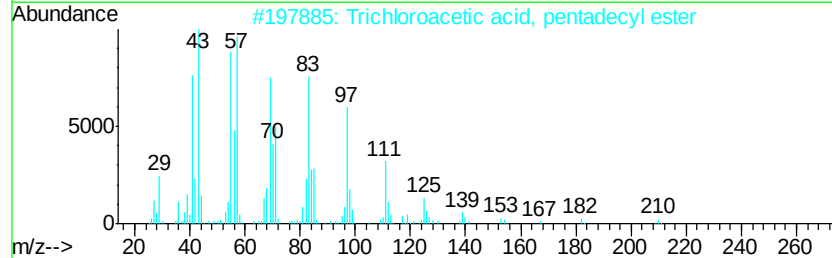
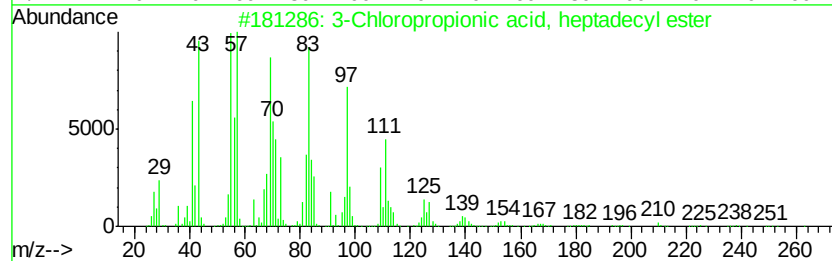
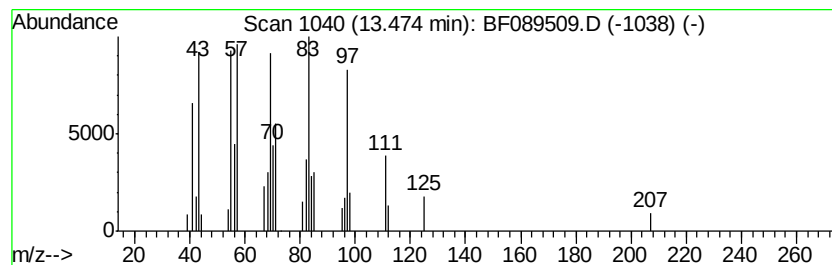
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Peak Number 6 3-Chloropropionic acid, hep... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	4.54 ng	57882	Chrysene-d12	13.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
2		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	91



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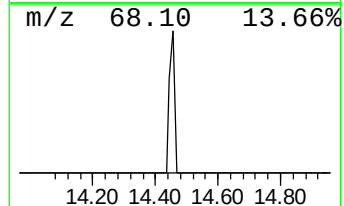
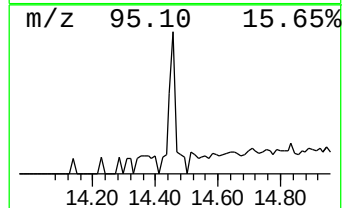
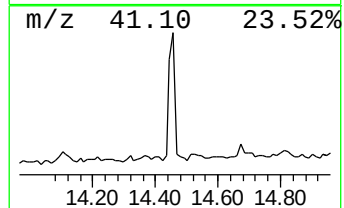
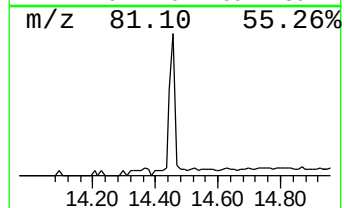
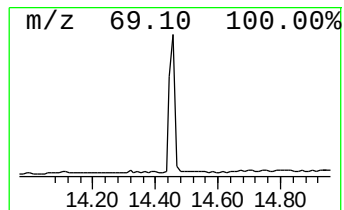
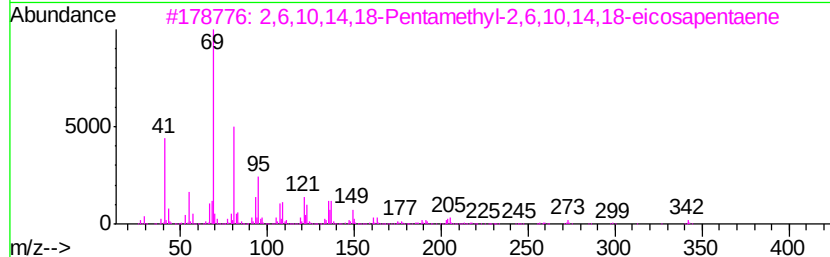
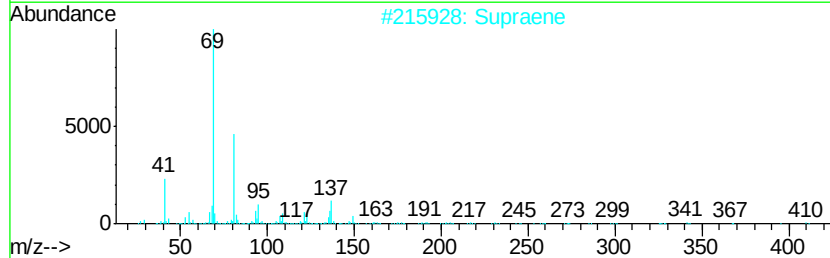
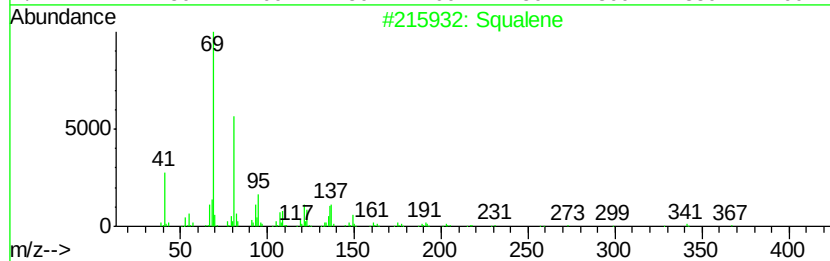
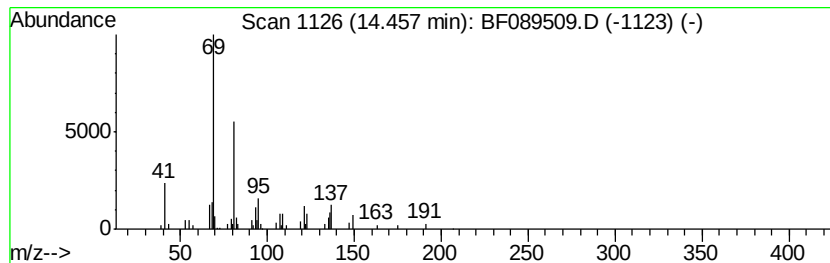
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Peak Number 7 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.46	7.32 ng	68308	Perylene-d12		14.93
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	90
4	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
5	trans-Farnesol	222	C15H26O	000106-28-5	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.57	33.0	ng	387216	1	6.48	234578	20.0
unknown6.25	6.25	115.4	ng	1353240	1	6.48	234578	20.0
Nonadecane	10.43	2.4	ng	41586	4	10.98	344919	20.0
3-Chloropropionic...	13.47	4.5	ng	57882	5	13.60	254931	20.0
Squalene	14.46	7.3	ng	68308	6	14.93	186562	20.0