

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092716\
 Data File : BF090261.D
 Acq On : 27 Sep 2016 19:32
 Operator : UM/SJ
 Sample : H4962-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BROOKLYN09

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-BF092016.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	1.644	4	5	52	rVB	2293235	6164965	100.00%	17.142%
2	4.559	258	260	270	rVB	345473	608535	9.87%	1.692%
3	5.039	299	302	304	rBV	2366468	2829308	45.89%	7.867%
4	6.136	395	398	400	rBV	2532927	2991787	48.53%	8.319%
5	6.239	404	407	410	rVB	2606565	2699253	43.78%	7.506%
6	6.467	425	427	430	rBV	605562	832005	13.50%	2.313%
7	6.627	439	441	444	rBV	2265757	2234578	36.25%	6.214%
8	7.050	475	478	480	rBV	1870583	2019956	32.77%	5.617%
9	7.759	538	540	543	rBV	1216076	1120151	18.17%	3.115%
10	8.845	632	635	637	rBV	3350153	3618374	58.69%	10.061%
11	9.245	667	670	672	rBV	1044232	1035282	16.79%	2.879%
12	9.496	690	692	695	rVB	1200590	1228918	19.93%	3.417%
13	9.965	731	733	734	rVB	113497	101738	1.65%	0.283%
14	10.182	748	752	753	rBV	52939	77840	1.26%	0.216%
15	10.285	758	761	763	rBV	1865983	1905972	30.92%	5.300%
16	10.433	772	774	778	rBV	137034	195838	3.18%	0.545%
17	10.879	811	813	814	rBV	61043	68643	1.11%	0.191%
18	10.971	818	821	823	rBV	1077973	1218051	19.76%	3.387%
19	11.234	841	844	847	rBV	127179	194929	3.16%	0.542%
20	11.531	868	870	873	rBV3	100893	140703	2.28%	0.391%
21	12.159	923	925	928	rBV	92845	103455	1.68%	0.288%
22	12.388	943	945	950	rVB	92162	110578	1.79%	0.307%
23	12.548	957	959	962	rBV	2054893	2365384	38.37%	6.577%
24	13.462	1037	1039	1044	rVB	201333	246450	4.00%	0.685%
25	13.577	1046	1049	1056	rBV	864410	961057	15.59%	2.672%
26	14.560	1132	1135	1138	rBV	45776	97448	1.58%	0.271%
27	14.891	1162	1164	1167	rBV	627426	791911	12.85%	2.202%

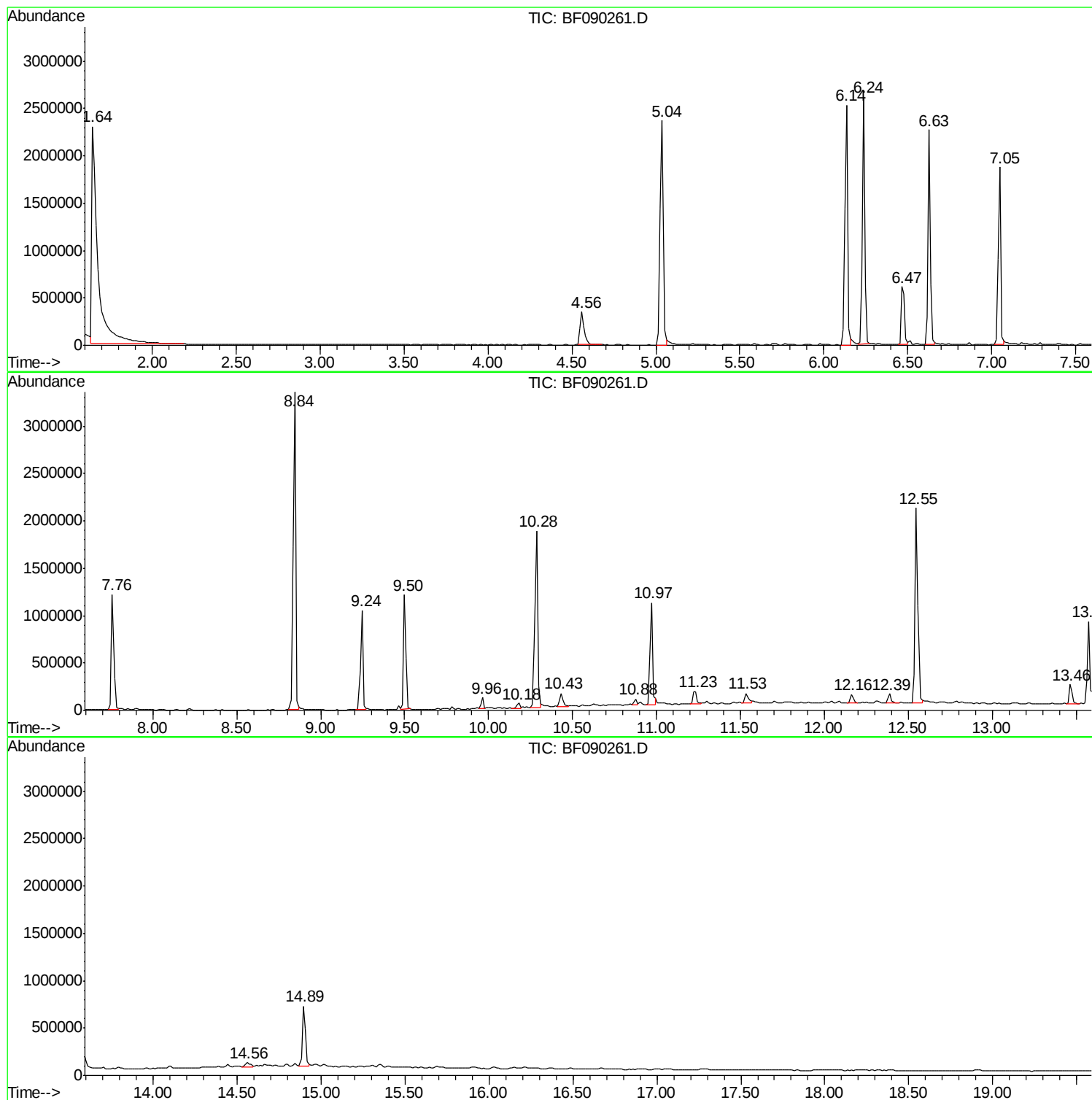
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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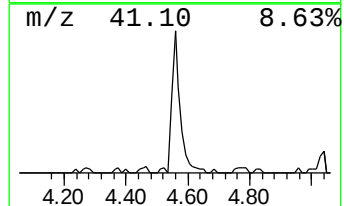
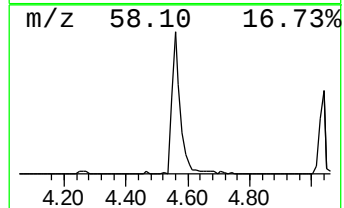
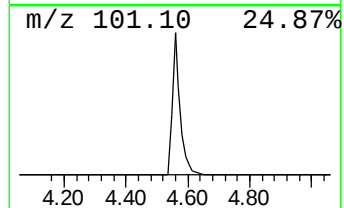
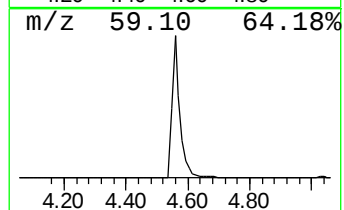
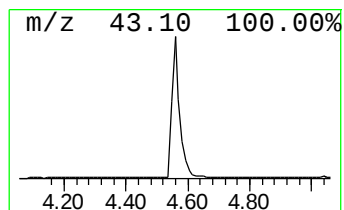
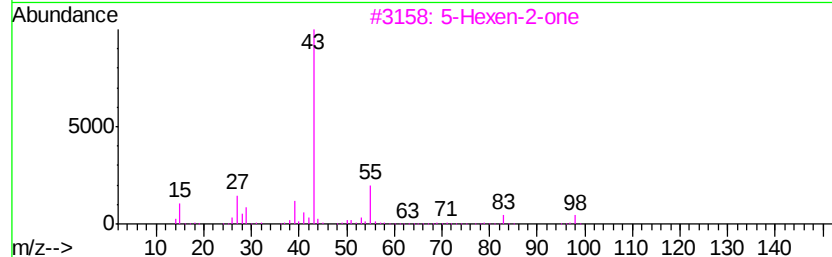
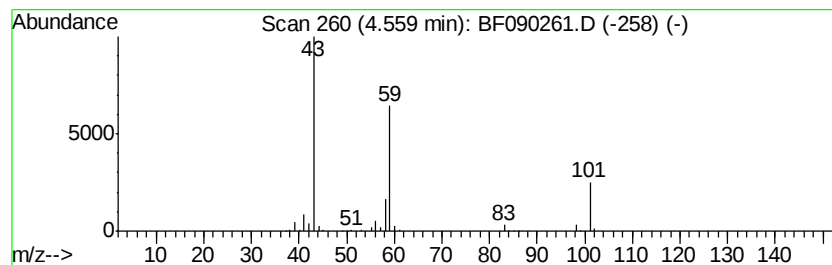
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.56	14.63 ng	608535	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	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		Acetone	58	C3H6O	000067-64-1	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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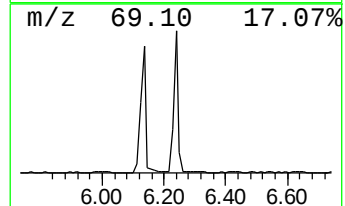
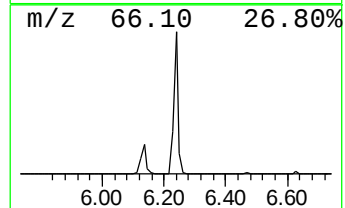
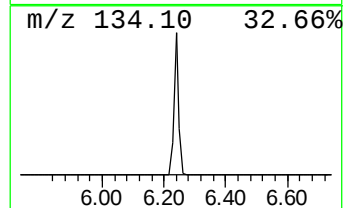
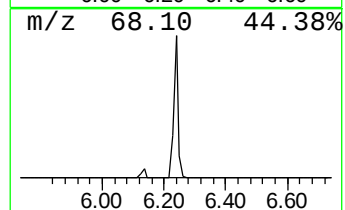
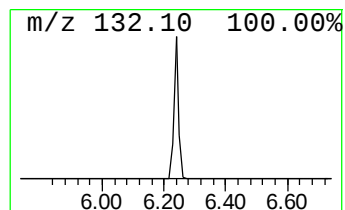
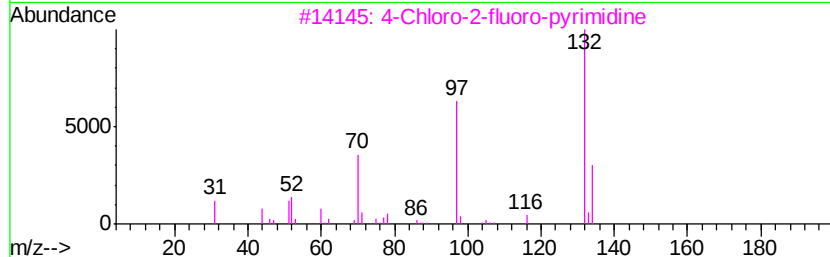
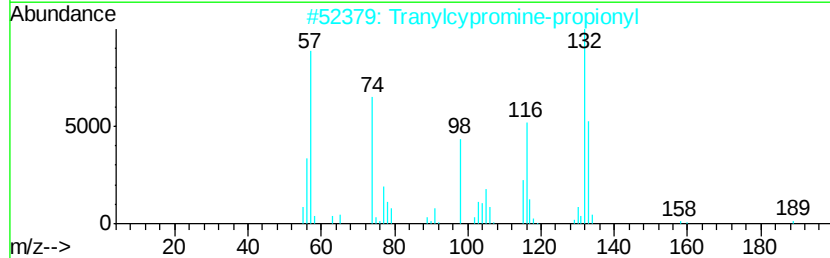
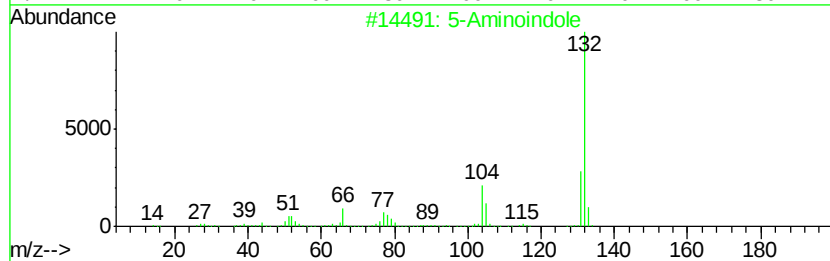
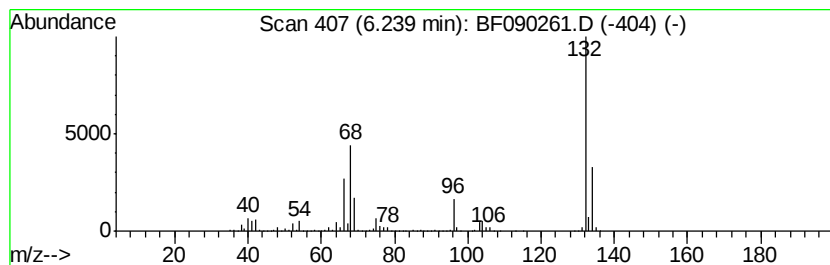
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Peak Number 3 unknown6.24 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.24	64.89 ng	2699250	1,4-Dichlorobenzene-d4	6.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	12
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9



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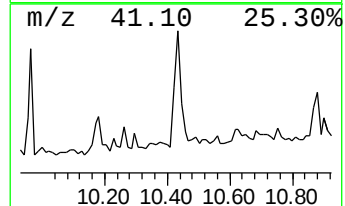
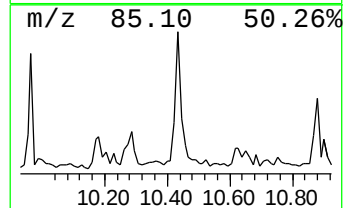
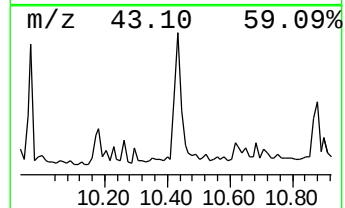
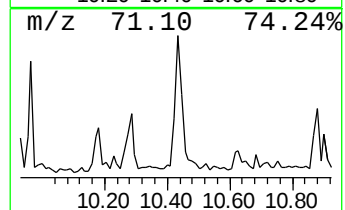
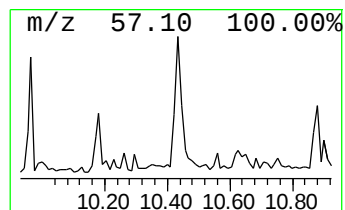
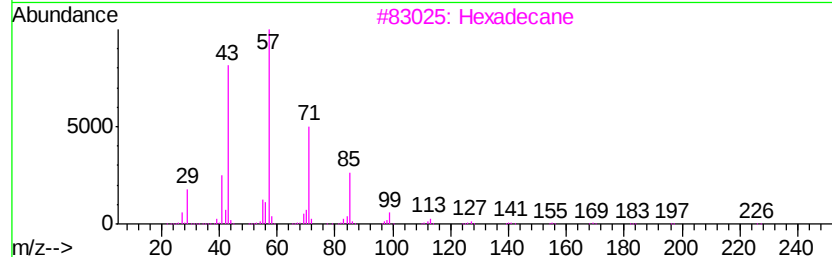
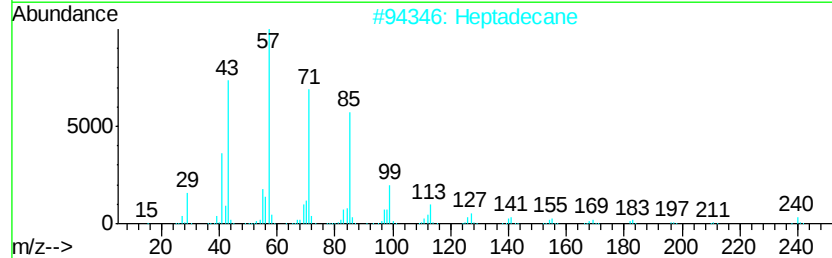
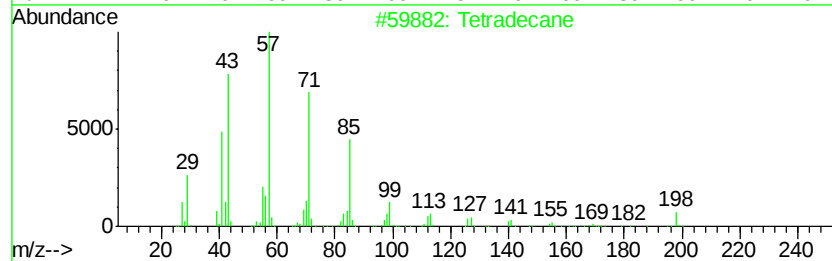
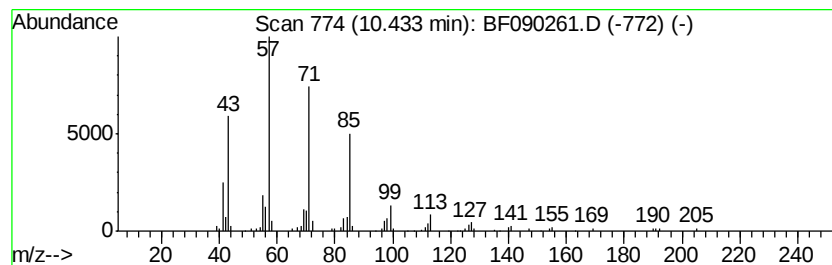
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Peak Number 5 Tetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.43	3.22 ng	195838	Phenanthrene-d10		10.97
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Hexadecane	226	C16H34	000544-76-3	90
4	Tetracosane	338	C24H50	000646-31-1	86
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86



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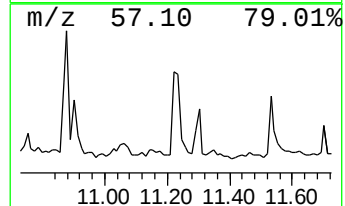
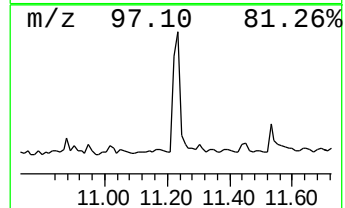
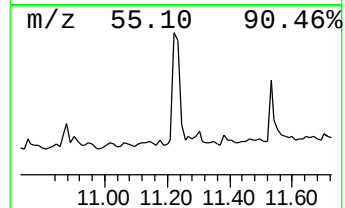
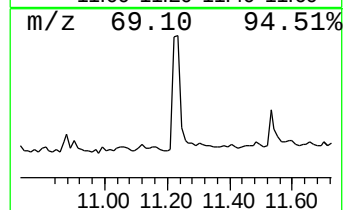
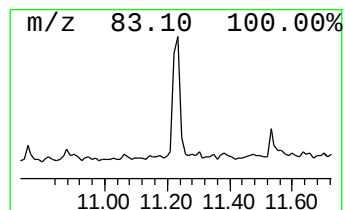
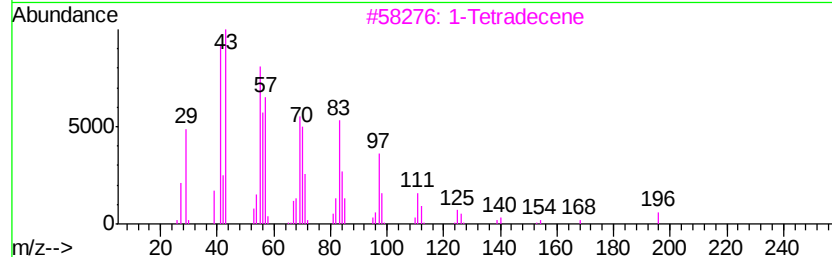
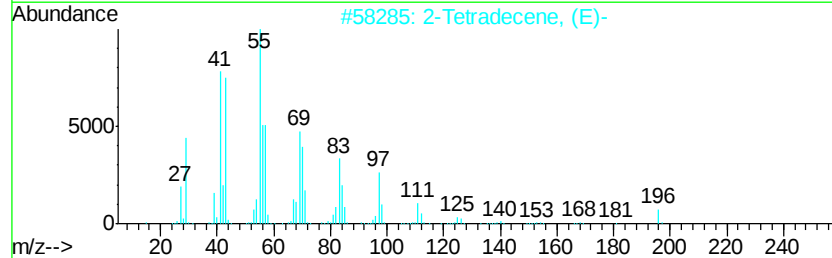
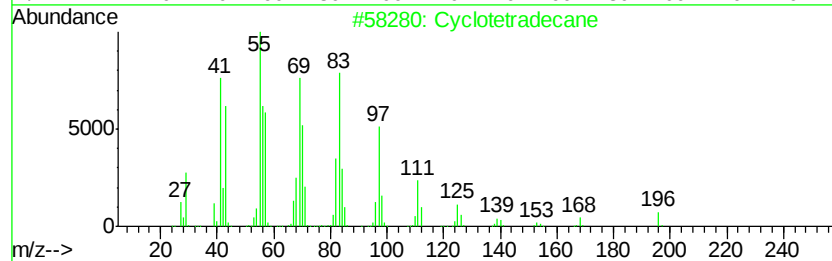
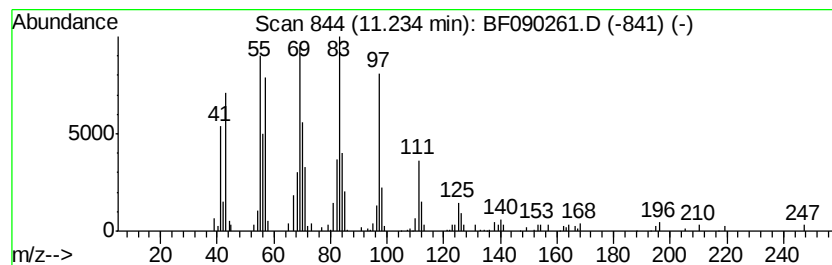
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Peak Number 6 Cyclotetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.23	3.20 ng	194929	Phenanthrene-d10	10.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclotetradecane	196	C14H28	000295-17-0	98
2		2-Tetradecene, (E)-	196	C14H28	035953-54-9	97
3		1-Tetradecene	196	C14H28	001120-36-1	97
4		1-Pentadecene	210	C15H30	013360-61-7	96
5		n-Pentadecanol	228	C15H32O	000629-76-5	95



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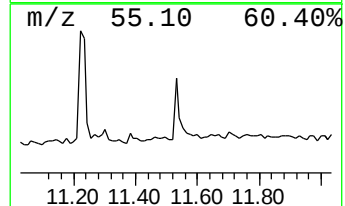
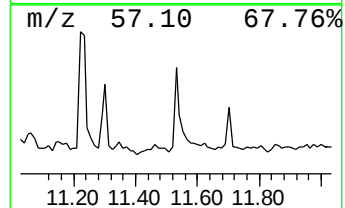
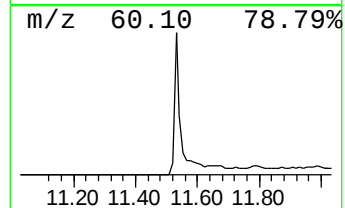
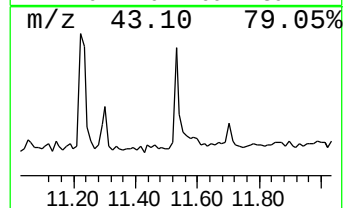
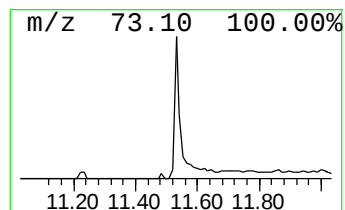
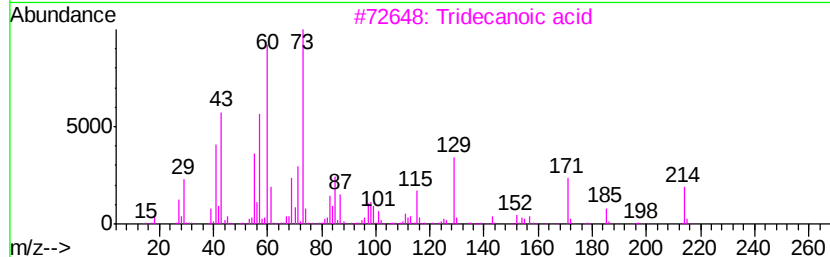
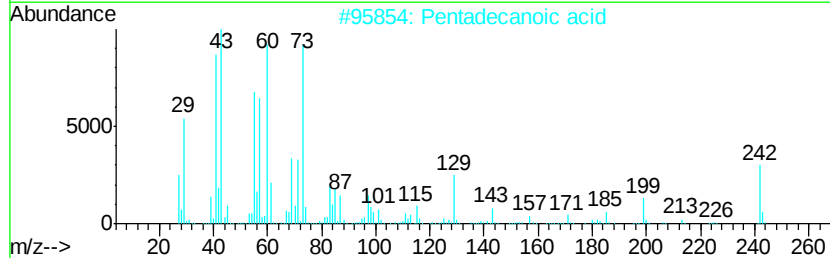
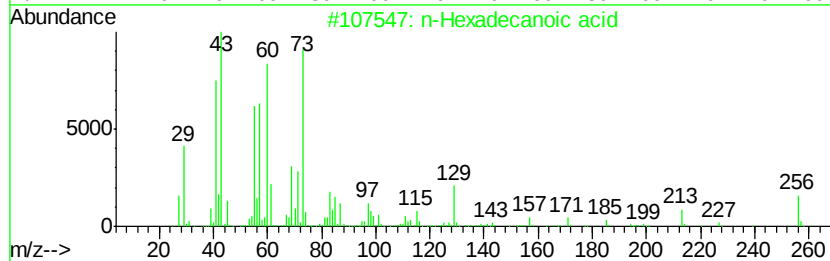
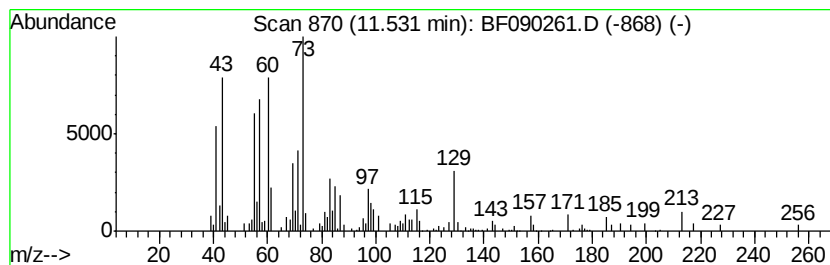
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Peak Number 7 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.53	2.31 ng	140703	Phenanthrene-d10	10.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81	
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80	
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72	
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64	
5	n-Decanoic acid	172	C10H20O2	000334-48-5	43	



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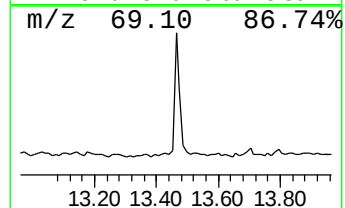
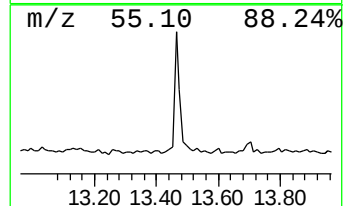
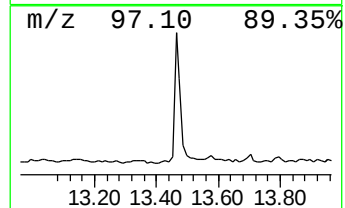
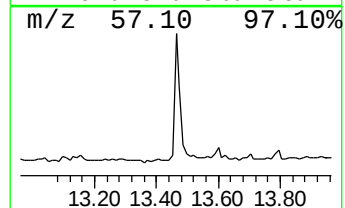
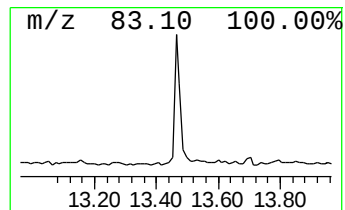
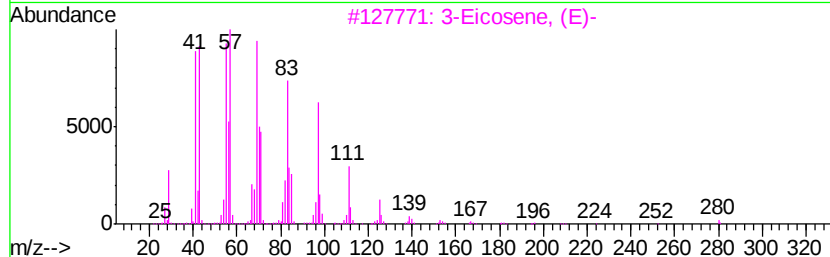
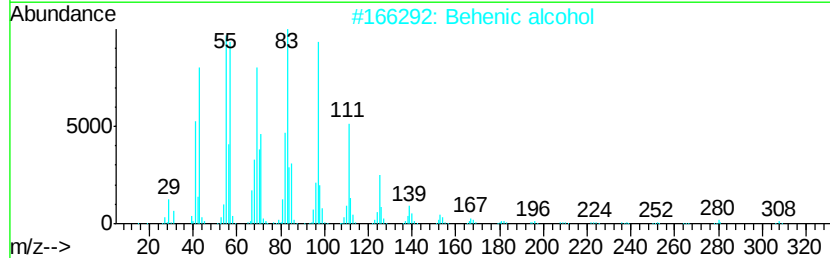
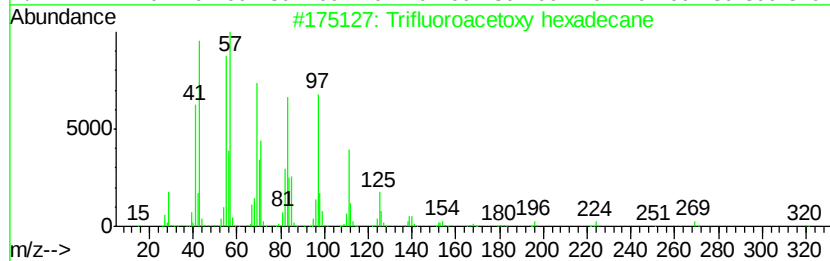
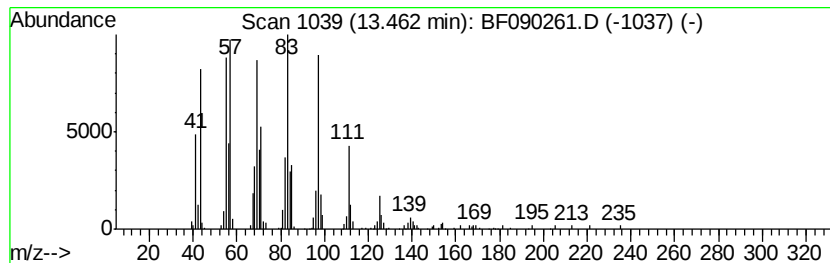
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.46	5.13 ng	246450	Chrysene-d12	13.58

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2		Behenic alcohol	326	C22H46O	000661-19-8	91
3		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4		1-Heneicosanol	312	C21H44O	015594-90-8	91
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092716\
Data File : BF090261.D
Acq On : 27 Sep 2016 19:32
Operator : UM/SJ
Sample : H4962-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BROOKLYN09

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.56	14.6	ng	608535	1	6.48	832005	20.0
unknown6.24	6.24	64.9	ng	2699250	1	6.48	832005	20.0
Tetradecane	10.43	3.2	ng	195838	4	10.97	1218050	20.0
Cyclotetradecane	11.23	3.2	ng	194929	4	10.97	1218050	20.0
n-Hexadecanoic acid	11.53	2.3	ng	140703	4	10.97	1218050	20.0
Trifluoroacetoxy ...	13.46	5.1	ng	246450	5	13.58	961057	20.0