LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088147.D
Acq On : 18 Jun 2016 21:30
Operator : UM/SJ
Sample : H3580-13
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B5(8-16)C

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	1.667	5	7	13	rVV	31536	48354	2.53%	0.262%
2	1.781	15	17	24	rVV	288204	398737	20.85%	2.157%
3	1.884	24	26	40	rVB	53974	93534	4.89%	0.506%
4	4.844	283	285	293	rVB	75294	110173	5.76%	0.596%
5	5.290	321	324	326	rBV	1714891	1911974	100.00%	10.344%
6	5.919	378	379	383	rVB2	11451	21603	1.13%	0.117%
7	6.010	383	387	390	rBV3	10688	30262	1.58%	0.164%
8	6.342	413	416	419	rBV2	1639466	1802903	94.30%	9.754%
9	6.456	423	426	429	rVB	1783329	1712293	89.56%	9.264%
10	6.536	431	433	435	rVB2	19588	30941	1.62%	0.167%
11	6.616	435	440	442	rBV3	13950	38290	2.00%	0.207%
12	6.684	444	446	449	rVB	677361	569236	29.77%	3.080%
13	6.776	449	454	456	rBV4	14261	40848	2.14%	0.221%
14	6.844	458	460	462	rBV	1565970	1592971	83.32%	8.618%
15	6.959	468	470	473	rVB2	12298	22443	1.17%	0.121%
16	7.107	481	483	487	rBV4	12441	25769	1.35%	0.139%
17	7.256	493	496	498	rBV	1120009	1114209	58.28%	6.028%
18	7.382	504	507	512	rVB2	23224	41796	2.19%	0.226%
19	7.610	523	527	529	rVB3	10721	23880	1.25%	0.129%
20	7.725	535	537	541	rVB2	13734	24219	1.27%	0.131%
21	7.896	546	552	554	rBV3	10131	30371	1.59%	0.164%
22	7.976	556	559	561	rBV	565007	678559	35.49%	3.671%
23	8.410	594	597	601	rBV2	17707	39169	2.05%	0.212%
24	9.005	646	649	650	rVB	15693	20491	1.07%	0.111%
25	9.050	650	653	655	rBV	2116263	1857286	97.14%	10.048%
26	9.450	685	688	690	rBV	701898	610599	31.94%	3.303%
27	9.668	705	707	709	rBV	40994	38990	2.04%	0.211%
28	9.725	709	712	714	rBV	641442	655003	34.26%	3.544%
29	10.159	749	750	752	rVB	65206	56308	2.95%	0.305%
30	10.376	766	769	773	rBV	29440	52920	2.77%	0.286%
31	10.513	778	781	783	rBV	766211	879480	46.00%	4.758%
32	10.639	790	792	796	rBV	58471	105945	5.54%	0.573%
33	10.833	806	809	813	rVB3	9572	23183	1.21%	0.125%
34	11.085	829	831	832	rBV	25912	37253	1.95%	0.202%

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.199	839	841	843	rBV	679073	604877	31.64%	3.272%
36	11.279	845	848	850	rVB	12686	22486	1.18%	0.122%
37	11.439	859	862	866	rBV4	7678	23754	1.24%	0.129%
38	11.805	892	894	899	rVB3	17147	36376	1.90%	0.197%
39	12.045	914	915	920	rVB3	18571	20539	1.07%	0.111%
40	12.411	945	947	949	rBV	103491	102581	5.37%	0.555%
41	12.639	964	967	968	rBV	68698	108942	5.70%	0.589%
42	12.788	977	980	982	rVB	1116997	1349119	70.56%	7.299%
43	12.959	993	995	999	rVB2	14250	26693	1.40%	0.144%
44	13.028	999	1001	1003	rBV	23258	28942	1.51%	0.157%
45	13.588	1047	1050	1053	rBV5	12409	34508	1.80%	0.187%
46	13.702	1057	1060	1064	rVV4	29183	80106	4.19%	0.433%
47	13.828	1068	1071	1076	rVV	568071	637344	33.33%	3.448%
48	13.931	1078	1080	1082	rVB	27063	31677	1.66%	0.171%
49	14.662	1142	1144	1146	rBV	38100	47959	2.51%	0.259%
50	14.834	1157	1159	1163	rBV	39012	70535	3.69%	0.382%
51	15.165	1185	1188	1190	rVB	26028	39895	2.09%	0.216%
52	15.211	1190	1192	1198	rVB	342054	422619	22.10%	2.286%
53	16.525	1304	1307	1313	rBV3	22693	55282	2.89%	0.299%

Sum of corrected areas: 18484226

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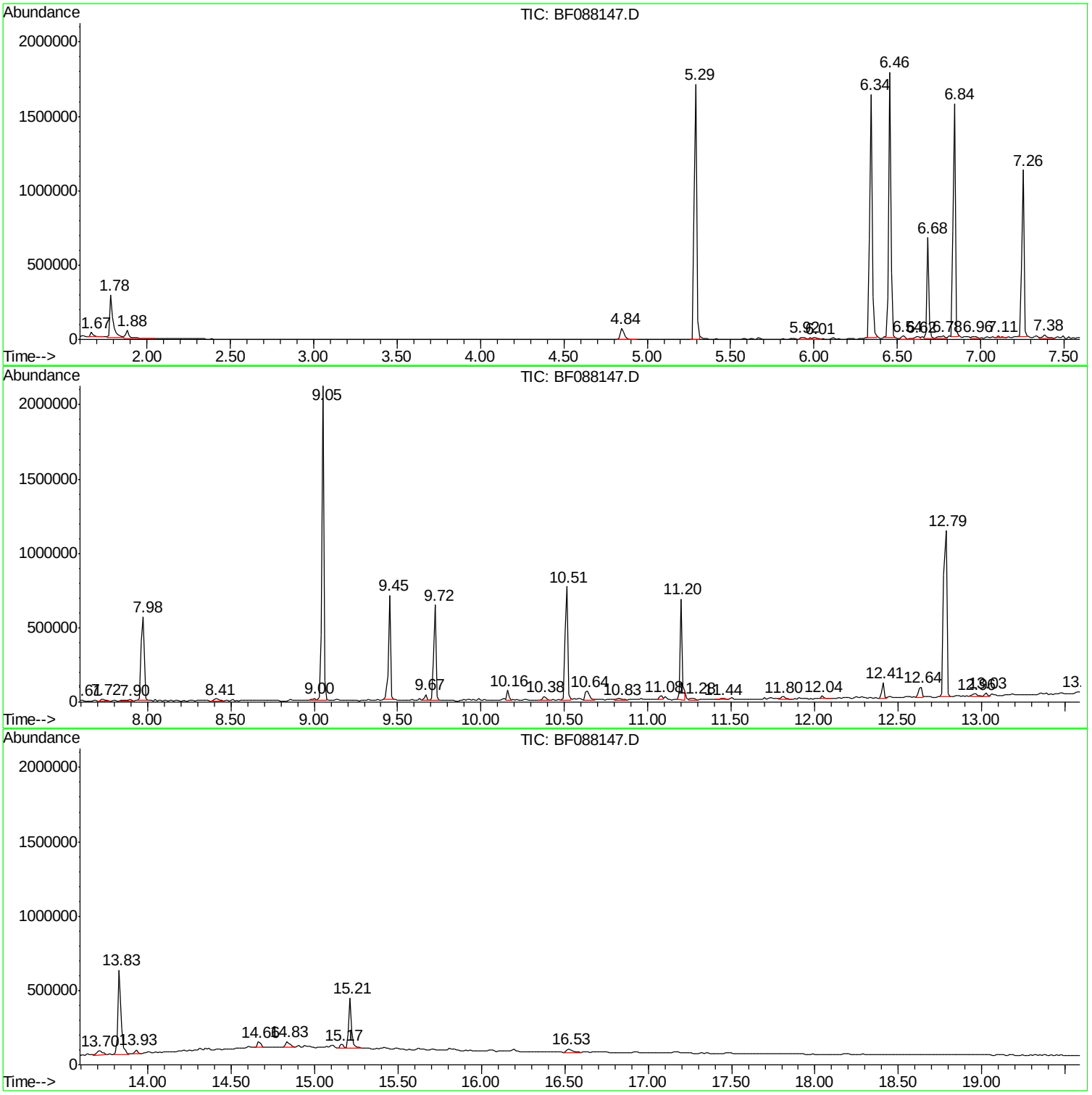
ClientSampleId :
08-B5(8-16)C

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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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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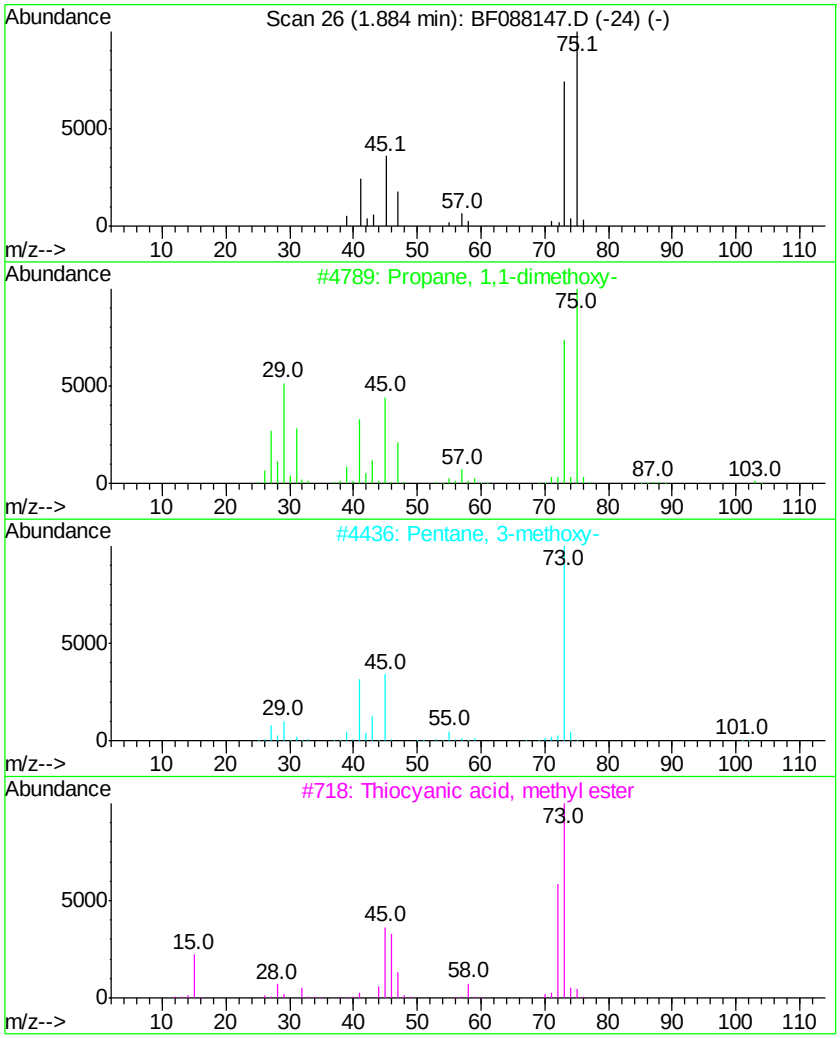
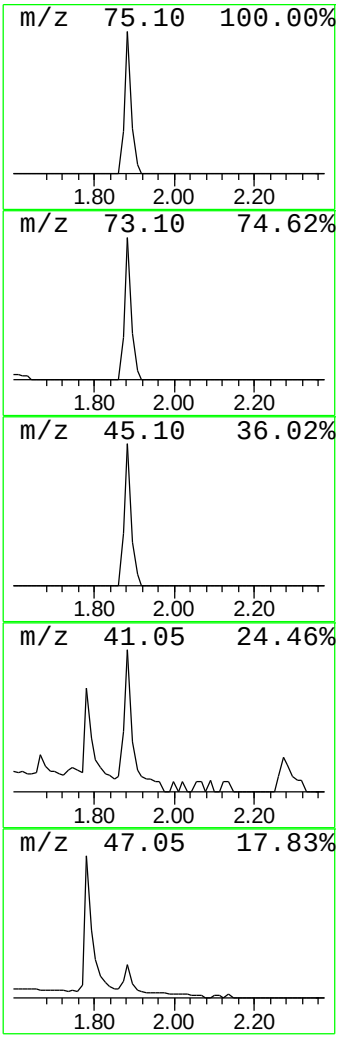
Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.88	3.29 ng	93534	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22
3	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	16
4	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	10
5	Glycine	75	C2H5NO2	000056-40-6	9





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Instrument : BNA_F
ClientSampleId : 08-B5(8-16)C

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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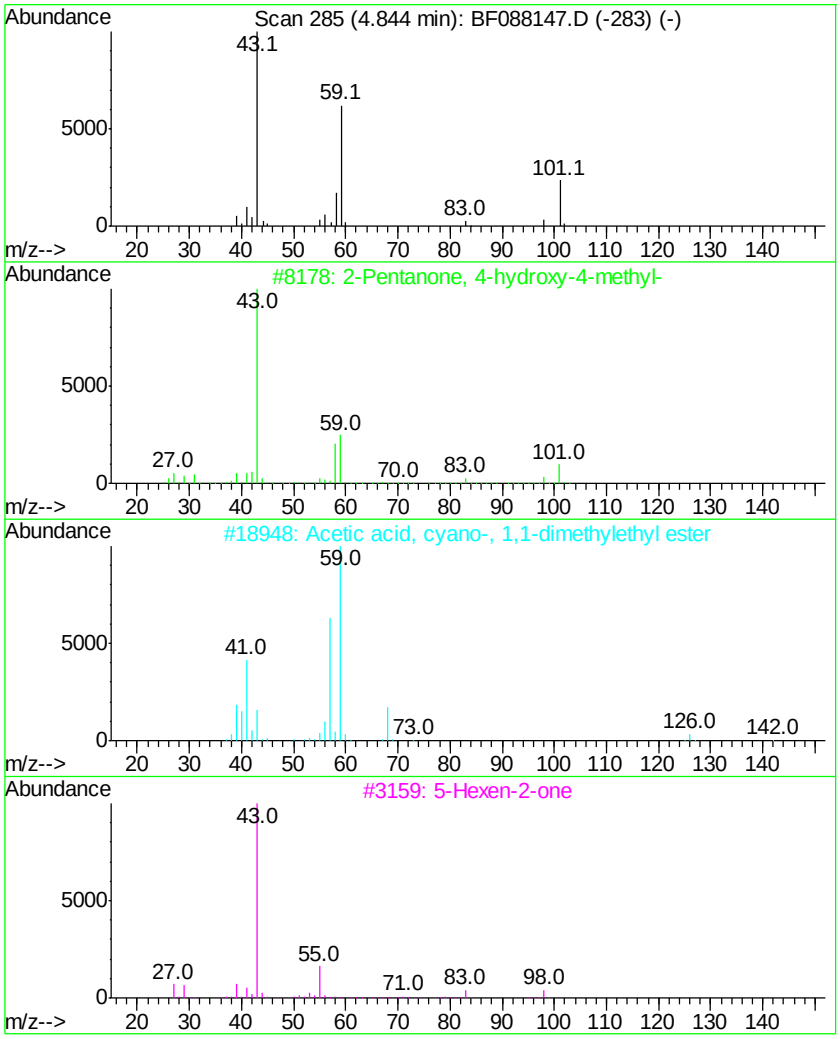
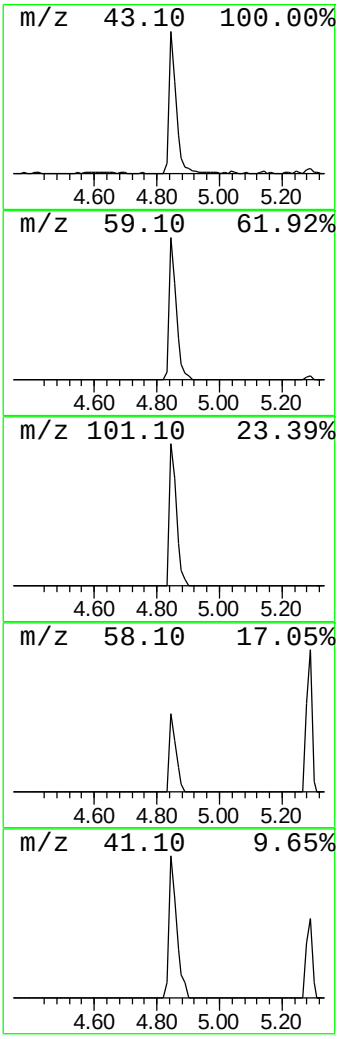
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	3.87 ng	110173	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Instrument : BNA_F
ClientSampleId : 08-B5(8-16)C

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
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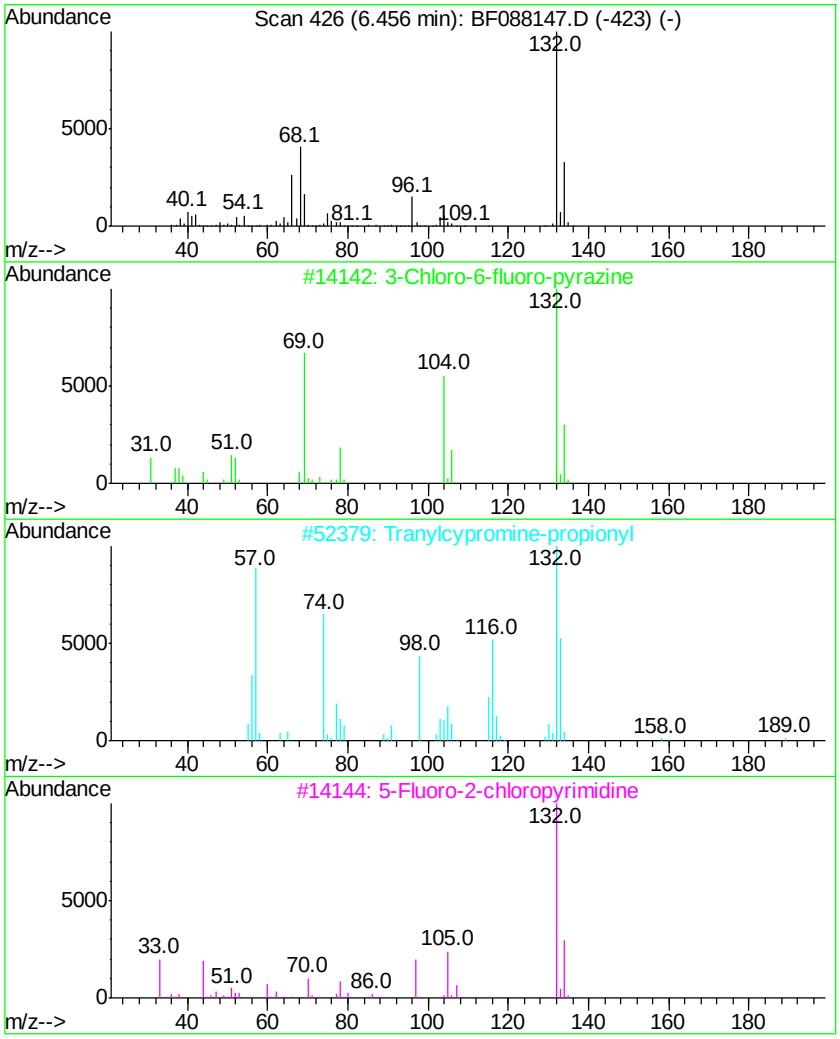
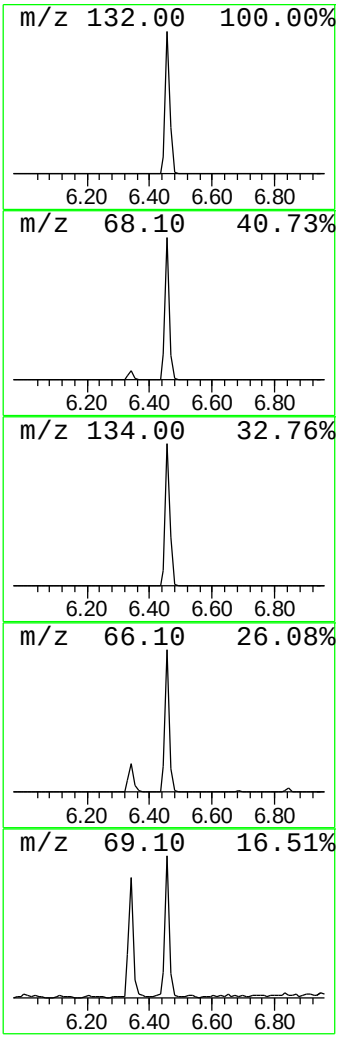
Peak Number 4 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	60.16 ng	1712290	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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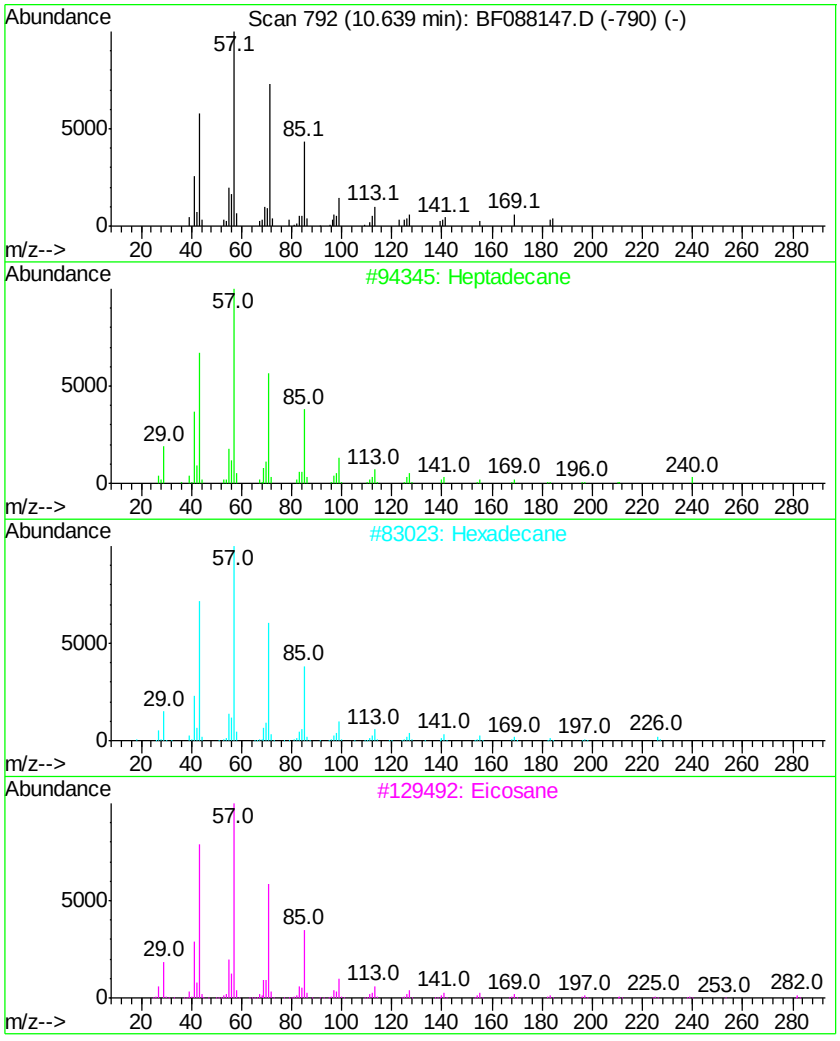
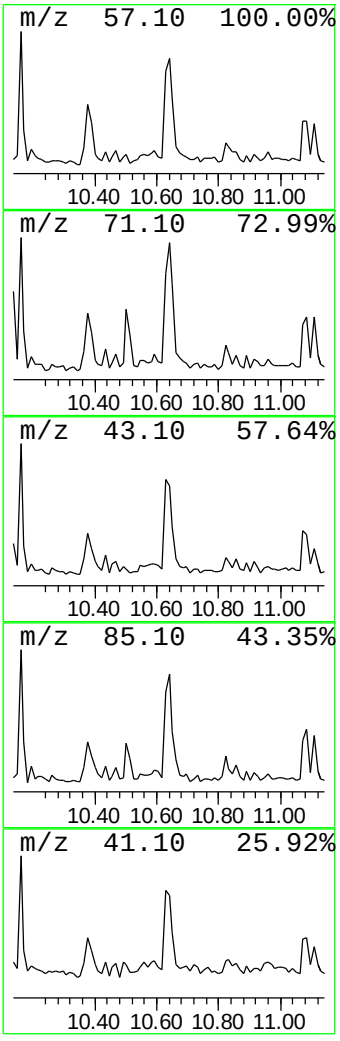
Peak Number 6 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.64	3.50 ng	105945	Phenanthrene-d10	11.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Eicosane	282	C20H42	000112-95-8	90
4	Octadecane	254	C18H38	000593-45-3	90
5	Tetracosane	338	C24H50	000646-31-1	86





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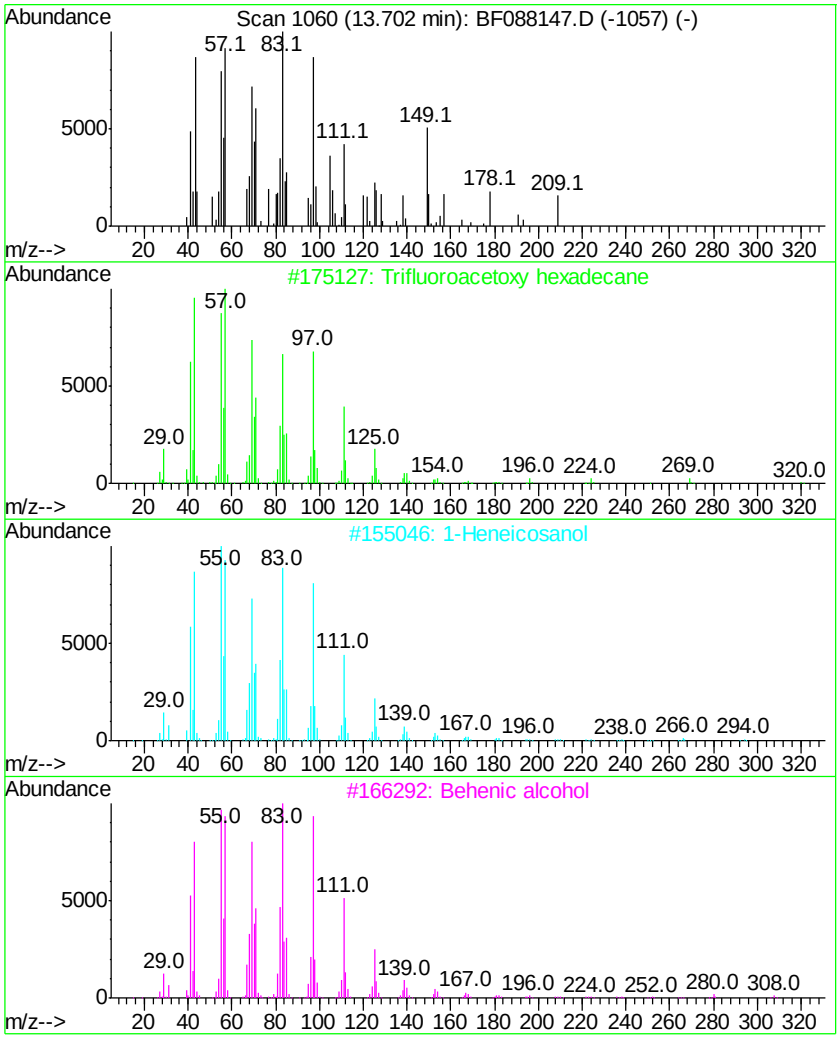
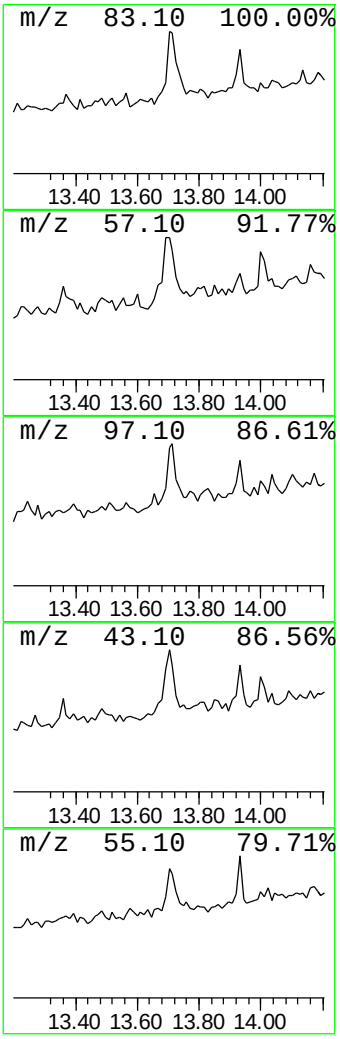
Peak Number 7 Trifluoroacetoxy hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	2.51 ng	80106	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	74
2	1-Heneicosanol	312	C21H44O	015594-90-8	74
3	Behenic alcohol	326	C22H46O	000661-19-8	74
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	72
5	1-Heptacosanol	396	C27H56O	002004-39-9	72





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TIC Library : C:\Database\NIST11.L
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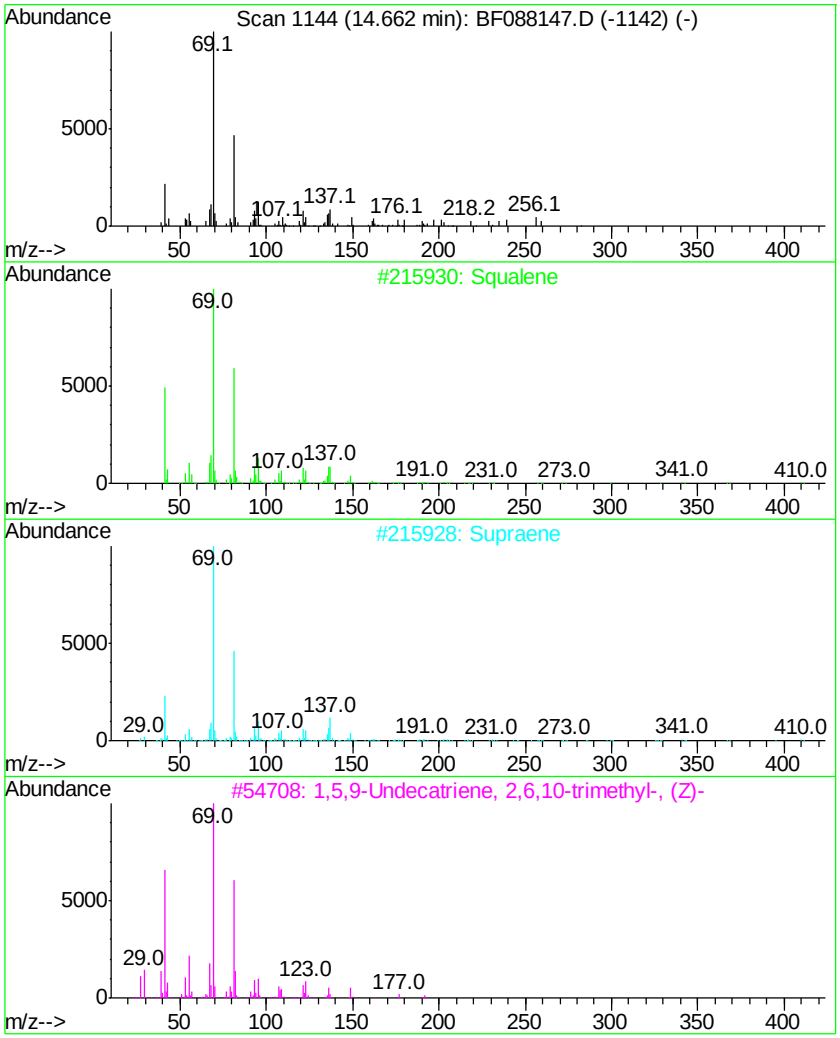
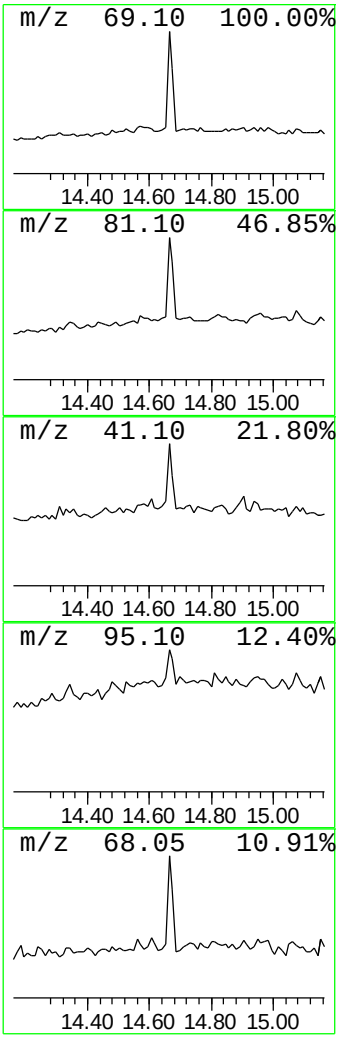
Peak Number 8 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	2.27 ng	47959	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	74
2	Supraene	410	C30H50	007683-64-9	72
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	59
4	4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	53
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	53





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 1,1-dime...	1.88	3.3	ng	93534	1	6.68	569236	20.0
2-Pentanone, 4-hy...	4.84	3.9	ng	110173	1	6.68	569236	20.0
unknown6.46	6.46	60.2	ng	1712290	1	6.68	569236	20.0
Heptadecane	10.64	3.5	ng	105945	4	11.20	604877	20.0
Trifluoroacetoxy ...	13.70	2.5	ng	80106	5	13.83	637344	20.0
Squalene	14.66	2.3	ng	47959	6	15.21	422619	20.0