LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071716\
Data File : BF089076.D
Acq On : 17 Jul 2016 14:12
Operator : UM/SJ
Sample : H4046-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C5-8

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-BF063016.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	13	rVB	60759	97997	5.93%	0.684%
2	1.758	13	15	40	rVB	577981	935649	56.65%	6.533%
3	4.799	279	281	288	rVB	65258	99611	6.03%	0.695%
4	5.244	318	320	323	rBV	975550	1395065	84.46%	9.740%
5	6.307	410	413	416	rBV	1145608	1322444	80.06%	9.233%
6	6.422	421	423	426	rBV	1196187	1461270	88.47%	10.203%
7	6.650	441	443	445	rVB	325464	336525	20.37%	2.350%
8	6.810	455	457	460	rBB	1248491	1093280	66.19%	7.633%
9	7.222	490	493	495	rBV	857452	863248	52.26%	6.027%
10	7.942	553	556	558	rBV	575783	509104	30.82%	3.555%
11	9.016	647	650	653	rVB	1284741	1651738	100.00%	11.532%
12	9.416	683	685	687	rVB	384757	310995	18.83%	2.171%
13	9.690	706	709	711	rBB	571837	549968	33.30%	3.840%
14	10.136	746	748	750	rVB	30263	22924	1.39%	0.160%
15	10.353	764	767	770	rBV	12473	20799	1.26%	0.145%
16	10.479	775	778	780	rVB	776896	932601	56.46%	6.511%
17	10.605	787	789	793	rVB	45673	51195	3.10%	0.357%
18	11.051	826	828	829	rBV	35058	29116	1.76%	0.203%
19	11.165	835	838	840	rBV	564137	507409	30.72%	3.543%
20	12.365	941	943	945	rBV	20334	16910	1.02%	0.118%
21	12.742	974	976	979	rVB	1009779	1250891	75.73%	8.734%
22	13.657	1053	1056	1061	rBV	66652	92542	5.60%	0.646%
23	13.782	1064	1067	1070	rBV	404343	372953	22.58%	2.604%
24	14.285	1109	1111	1115	rBV	13271	20860	1.26%	0.146%
25	14.628	1139	1141	1144	rBV	44783	58776	3.56%	0.410%
26	14.777	1152	1154	1158	rBV	10931	19810	1.20%	0.138%
27	15.142	1184	1186	1189	rVB	268409	298907	18.10%	2.087%

Sum of corrected areas: 14322587

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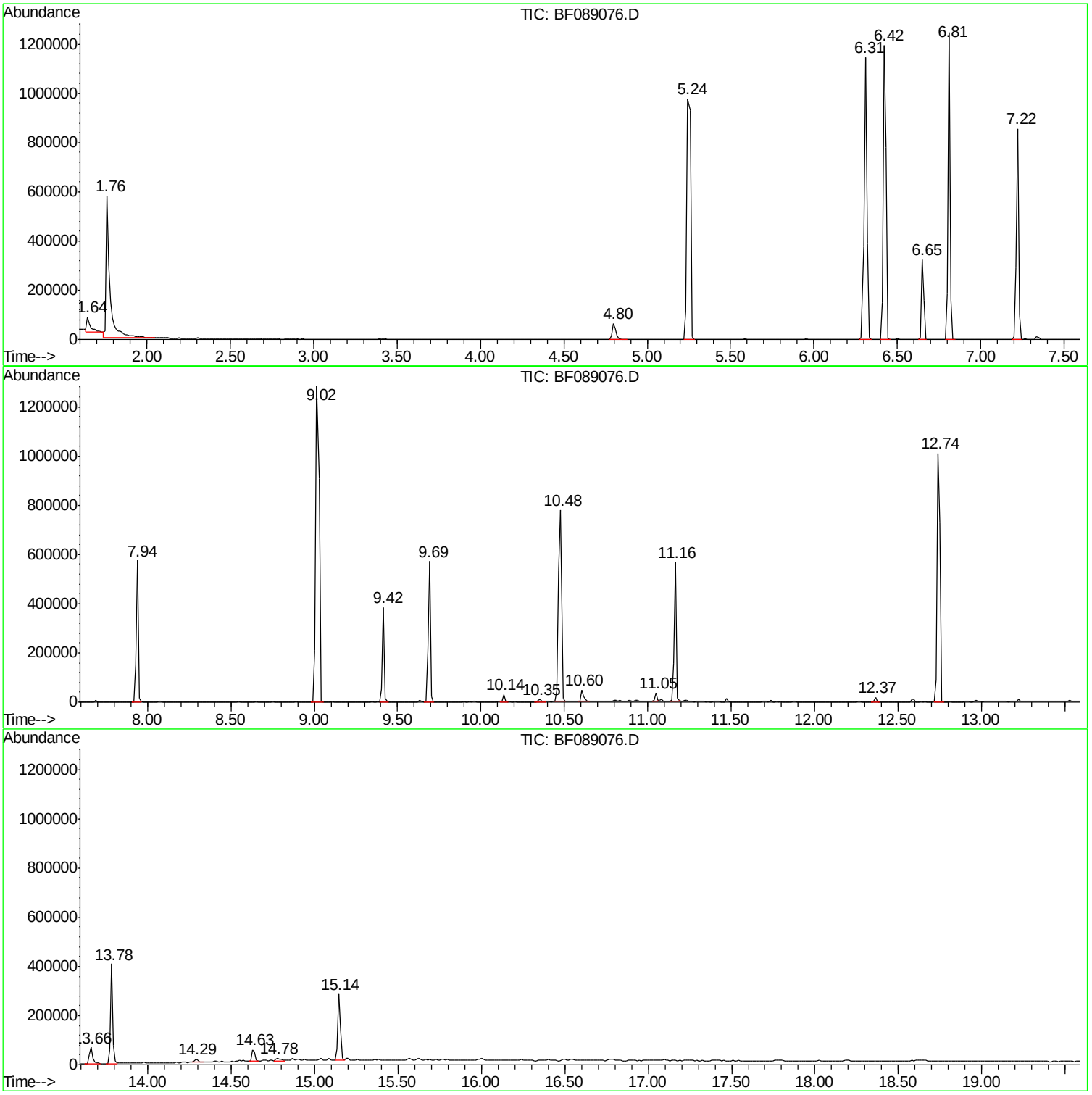
ClientSampleId :
C5-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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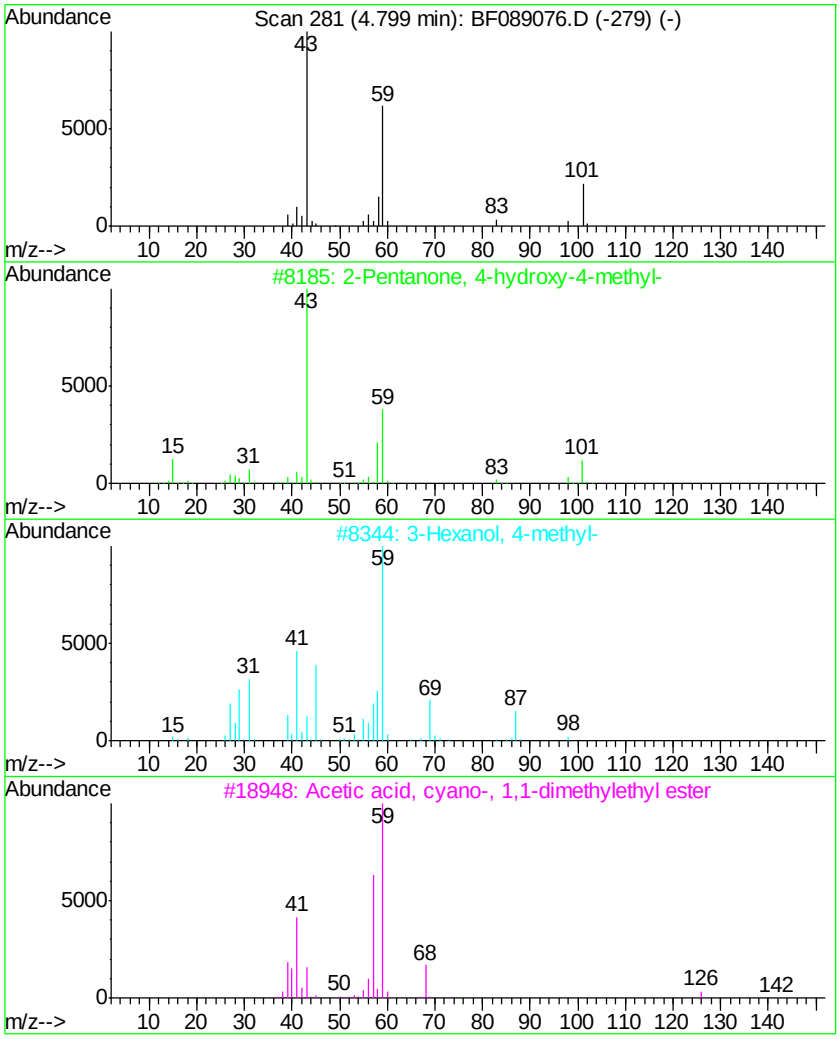
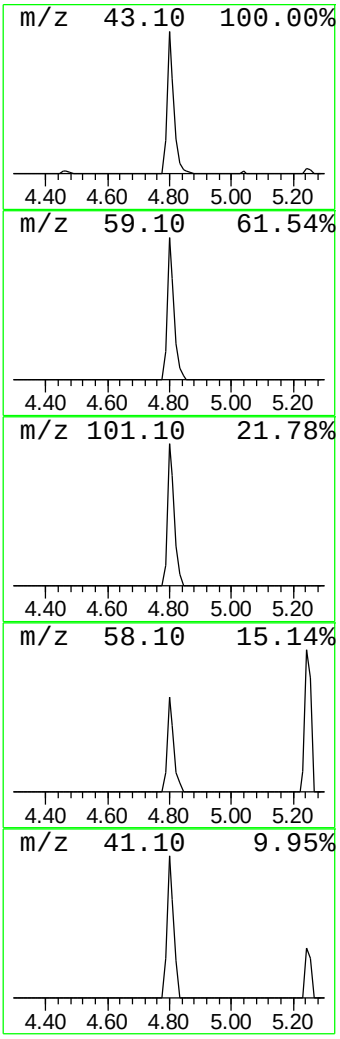
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	5.92 ng	99611	1,4-Dichlorobenzene-d4	6.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
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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ClientSampleId : C5-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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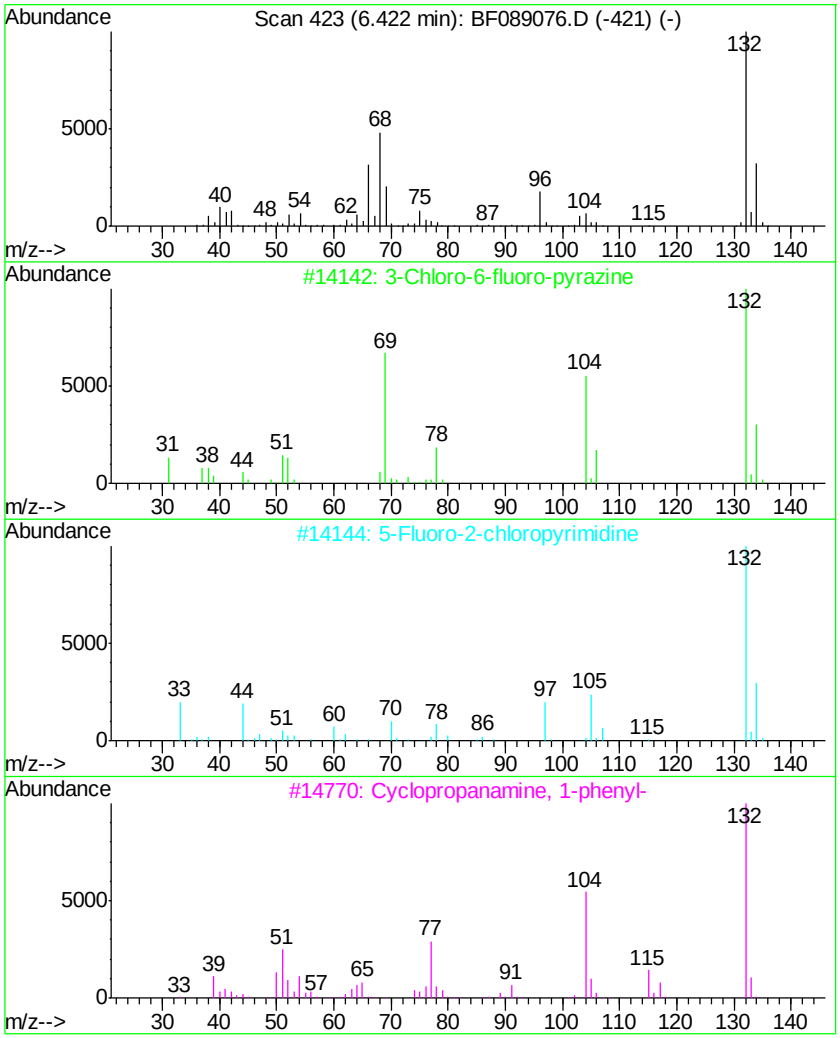
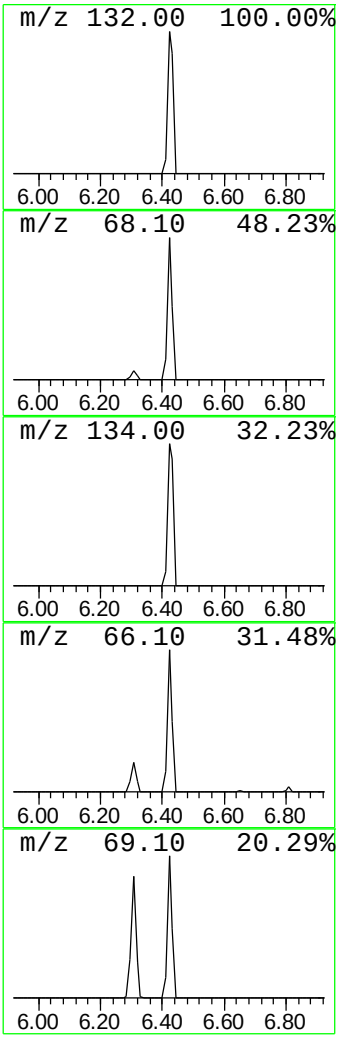
Peak Number 4 unknown6.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	86.84 ng	1461270	1,4-Dichlorobenzene-d4	6.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





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ClientSampleId : C5-8

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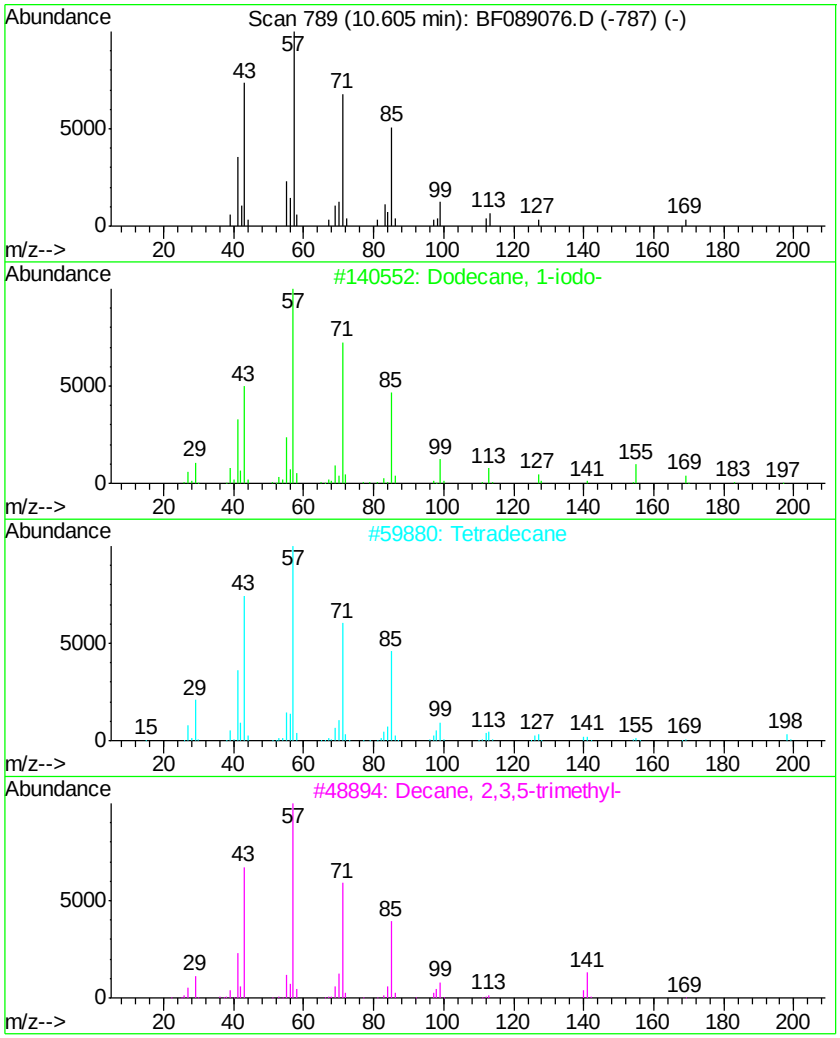
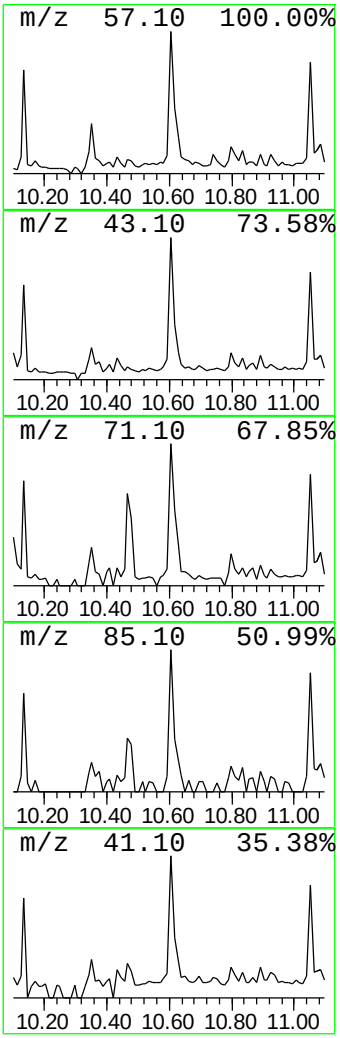
Peak Number 6 Dodecane, 1-iodo- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.60	2.02 ng	51195	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
2	Tetradecane	198	C14H30	000629-59-4	86
3	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	86
4	Tetracosane	338	C24H50	000646-31-1	80
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	80





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : C5-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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TIC Library : C:\Database\NIST11.L
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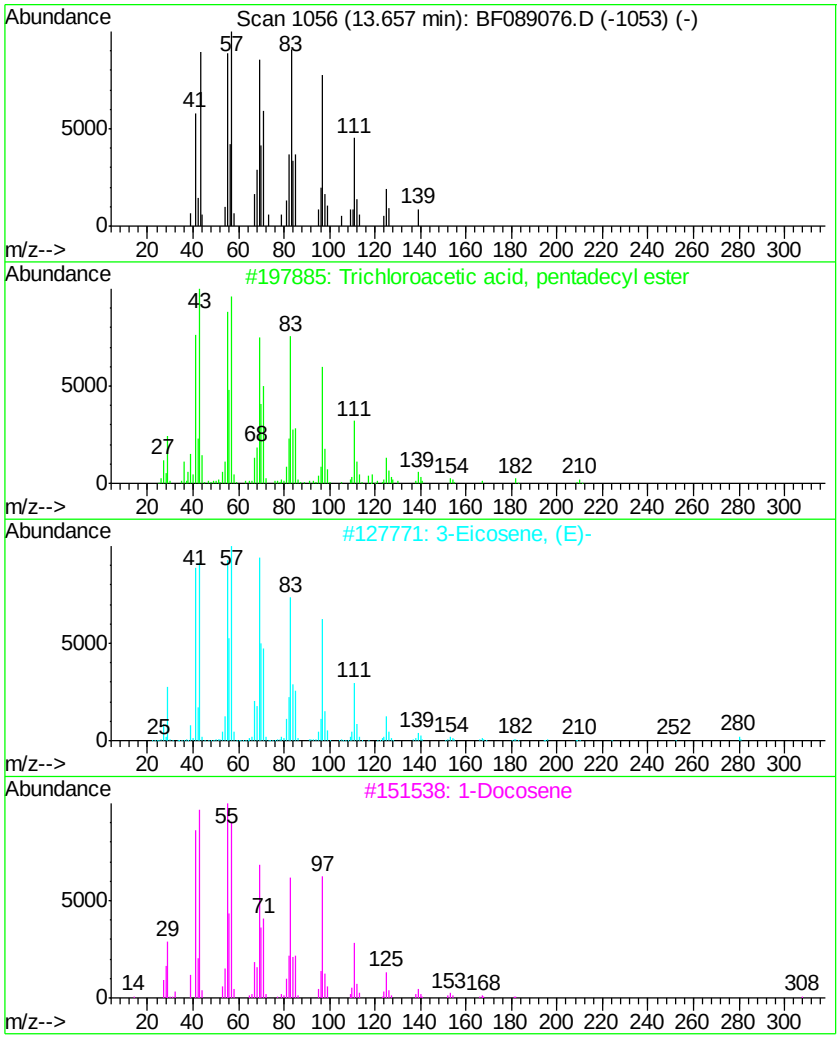
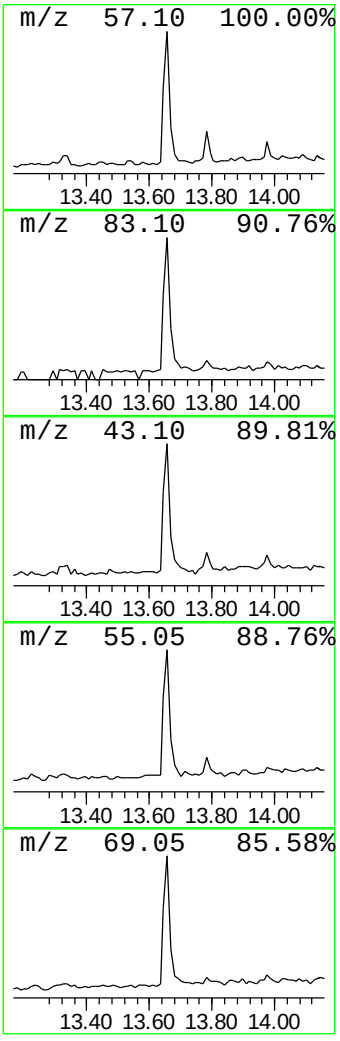
Peak Number 7 Trichloroacetic acid, penta... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.66	4.96 ng	92542	Chrysene-d12	13.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	1-Docosene	308	C22H44	001599-67-3	81
4	17-Pentatriacontene	491	C35H70	006971-40-0	80
5	11-Tricosene	322	C23H46	052078-56-5	72





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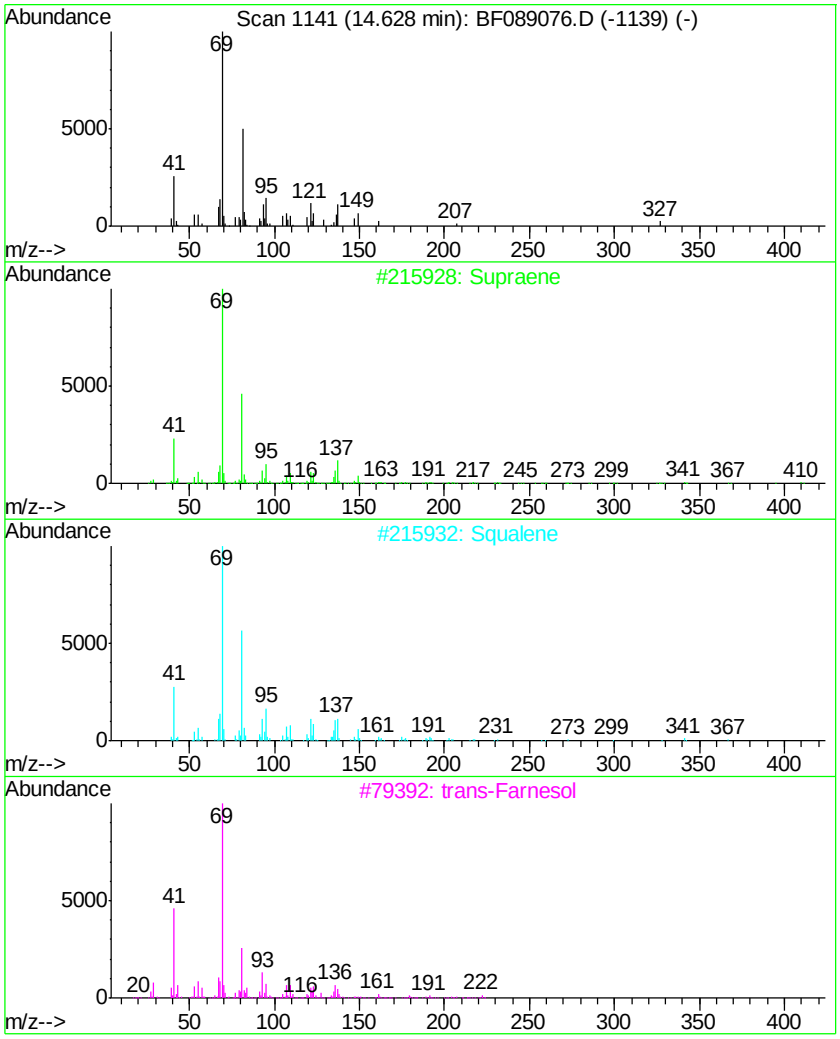
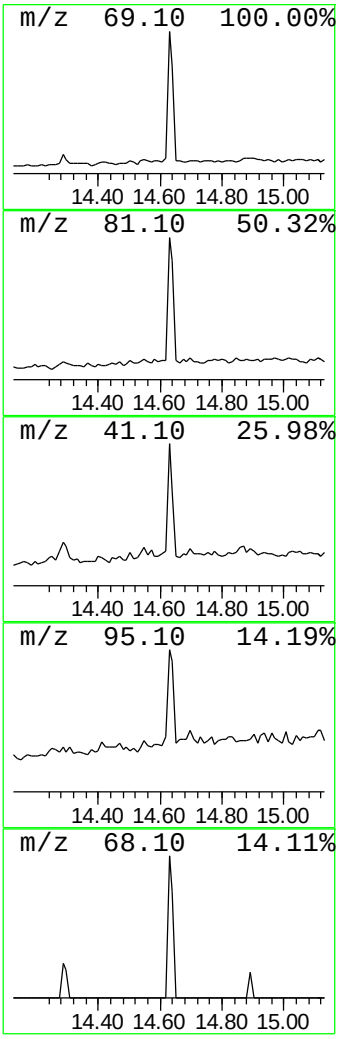
Peak Number 8 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	3.93 ng	58776	Perylene-d12	15.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	90
2	Squalene	410	C30H50	000111-02-4	80
3	trans-Farnesol	222	C15H26O	000106-28-5	59
4	2,2-Dimethyl-3-(3,7,16,20-tetram...	412	C29H48O	1000194-78-6	53
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	50





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.80	5.9	ng	99611	1	6.65	336525	20.0
unknown6.42	6.42	86.8	ng	1461270	1	6.65	336525	20.0
Dodecane, 1-iodo-	10.60	2.0	ng	51195	4	11.16	507409	20.0
Trichloroacetic a...	13.66	5.0	ng	92542	5	13.78	372953	20.0
Supraene	14.63	3.9	ng	58776	6	15.14	298907	20.0