LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092217\
Data File : BF098689.D
Acq On : 22 Sep 2017 10:16
Operator : SJ/JU
Sample : I5311-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-03-091917

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-BF092117.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	2.157	10	12	22	rVB2	78742	118658	3.82%	0.393%
2	2.234	22	25	43	rVB	103243	201592	6.49%	0.667%
3	2.357	44	46	60	rVB2	31387	57780	1.86%	0.191%
4	4.545	414	418	424	rBV	242716	257094	8.28%	0.851%
5	5.151	517	521	531	rBV	846082	969815	31.23%	3.209%
6	5.539	582	587	590	rBV	2548232	2438939	78.53%	8.069%
7	6.545	750	758	762	rBV	2708137	2955694	95.17%	9.779%
8	6.692	778	783	786	rBV	3088574	2842316	91.52%	9.404%
9	6.757	791	794	797	rBV2	54827	48198	1.55%	0.159%
10	6.928	819	823	826	rVB	1054564	885691	28.52%	2.930%
11	7.081	845	849	853	rBV	2433756	2149022	69.20%	7.110%
12	7.486	907	918	921	rBV	2137967	1942513	62.55%	6.427%
13	7.516	921	923	927	rVB	110630	83307	2.68%	0.276%
14	8.204	1037	1040	1043	rBV	1298010	1076298	34.66%	3.561%
15	9.280	1218	1223	1226	rBV	3680713	3105643	100.00%	10.275%
16	9.357	1233	1236	1238	rBV2	43370	38680	1.25%	0.128%
17	9.669	1286	1289	1293	rBV	287429	228938	7.37%	0.757%
18	9.822	1312	1315	1319	rBV	110299	91590	2.95%	0.303%
19	9.886	1321	1326	1329	rVB	47360	47239	1.52%	0.156%
20	9.963	1335	1339	1342	rVB	1148418	1020958	32.87%	3.378%
21	10.386	1408	1411	1413	rVB	67481	56788	1.83%	0.188%
22	10.604	1444	1448	1453	rVB2	40065	57562	1.85%	0.190%
23	10.745	1466	1472	1475	rBV	878242	762279	24.54%	2.522%
24	10.857	1488	1491	1500	rVB	94501	146600	4.72%	0.485%
25	11.045	1519	1523	1527	rBV7	24371	35314	1.14%	0.117%
26	11.304	1564	1567	1569	rBV	71026	52321	1.68%	0.173%
27	11.333	1569	1572	1579	rVB3	53823	64187	2.07%	0.212%
28	11.445	1587	1591	1593	rBV	1029961	820604	26.42%	2.715%
29	11.469	1593	1595	1599	rVV	204608	164802	5.31%	0.545%
30	11.521	1599	1604	1606	rVB	74788	78168	2.52%	0.259%
31	11.733	1636	1640	1643	rBV2	39652	37608	1.21%	0.124%
32	11.945	1673	1676	1678	rBV	41074	40570	1.31%	0.134%
33	11.974	1678	1681	1684	rVB	51457	51079	1.64%	0.169%
34	12.057	1692	1695	1698	rBV2	63539	67804	2.18%	0.224%

LSC Area Percent Report

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Acq On : 22 Sep 2017 10:16
Operator : SJ/JU
Sample : I5311-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-03-091917

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-BF092117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.492	1766	1769	1772	rBV	52135	49059	1.58%	0.162%
36	12.527	1772	1775	1777	rBV3	56503	55952	1.80%	0.185%
37	12.574	1781	1783	1787	rBV2	35864	43642	1.41%	0.144%
38	12.657	1794	1797	1801	rVB	500966	404710	13.03%	1.339%
39	12.751	1810	1813	1816	rBV	61608	58381	1.88%	0.193%
40	12.810	1820	1823	1825	rBV	35772	38911	1.25%	0.129%
41	12.886	1830	1836	1840	rBV	509006	507701	16.35%	1.680%
42	13.027	1856	1860	1864	rVB	2497765	2152801	69.32%	7.123%
43	13.098	1869	1872	1877	rBV2	52046	79782	2.57%	0.264%
44	13.192	1885	1888	1889	rBV2	38881	43035	1.39%	0.142%
45	13.210	1889	1891	1894	rVB	96279	86199	2.78%	0.285%
46	13.280	1900	1903	1906	rVB	50662	43478	1.40%	0.144%
47	13.315	1906	1909	1913	rBV2	62795	73692	2.37%	0.244%
48	13.921	2009	2012	2015	rVB2	85931	93168	3.00%	0.308%
49	14.080	2035	2039	2042	rBV2	934743	1183783	38.12%	3.917%
50	14.110	2042	2044	2046	rVB	269431	203520	6.55%	0.673%
51	15.139	2215	2219	2227	rVB	376590	791312	25.48%	2.618%
52	15.515	2279	2283	2289	rBV	293911	428200	13.79%	1.417%
53	15.580	2290	2294	2298	rBV	663125	891296	28.70%	2.949%

Sum of corrected areas: 30224273

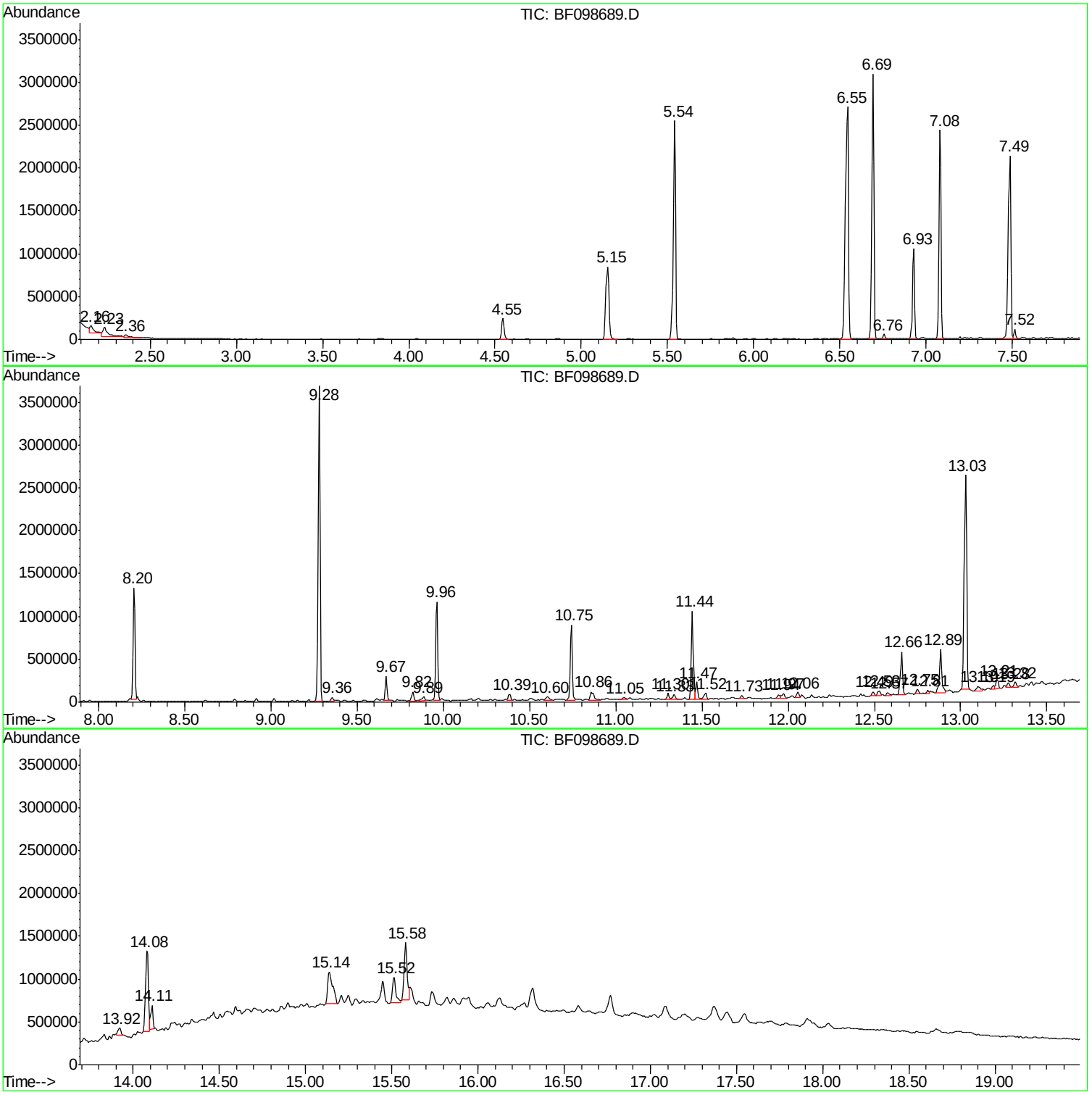
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092217\
Data File : BF098689.D
Acq On : 22 Sep 2017 10:16
Operator : SJ/JU
Sample : I5311-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-03-091917

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092217\
Data File : BF098689.D
Acq On : 22 Sep 2017 10:16
Operator : SJ/JU
Sample : I5311-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-03-091917

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

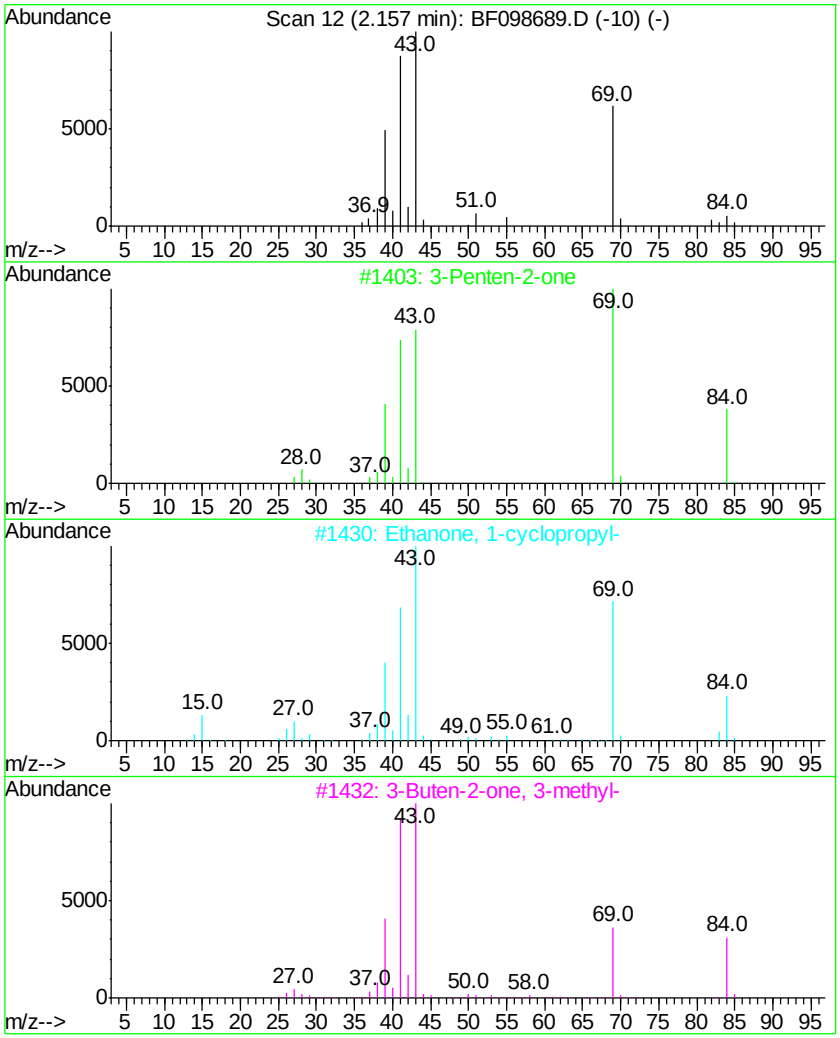
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

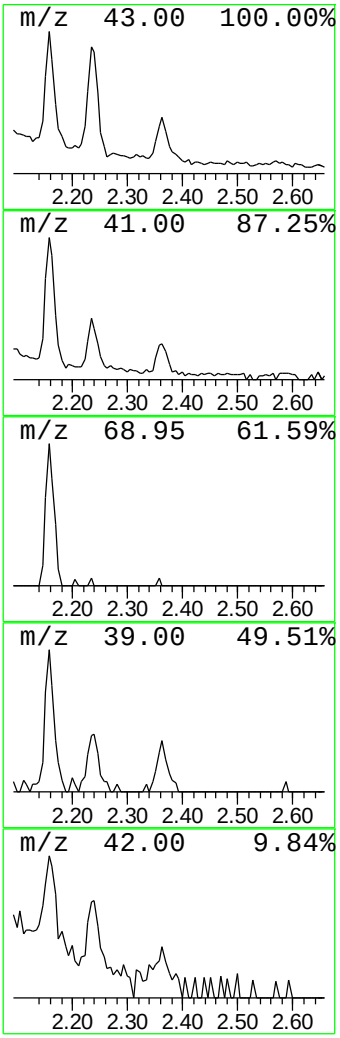
****

Peak Number 1 3-Penten-2-one Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	2.68 ng	118658	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one	84	C5H8O	000625-33-2	83
2	Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	78
3	3-Buten-2-one, 3-methyl-	84	C5H8O	000814-78-8	43
4	2-Butenal	70	C4H6O	004170-30-3	38
5	Cyclopropanecarboxylic acid, 5-f...	225	C10H8FNO4	1000278-66-5	33





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092217\
Data File : BF098689.D
Acq On : 22 Sep 2017 10:16
Operator : SJ/JU
Sample : I5311-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-03-091917

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

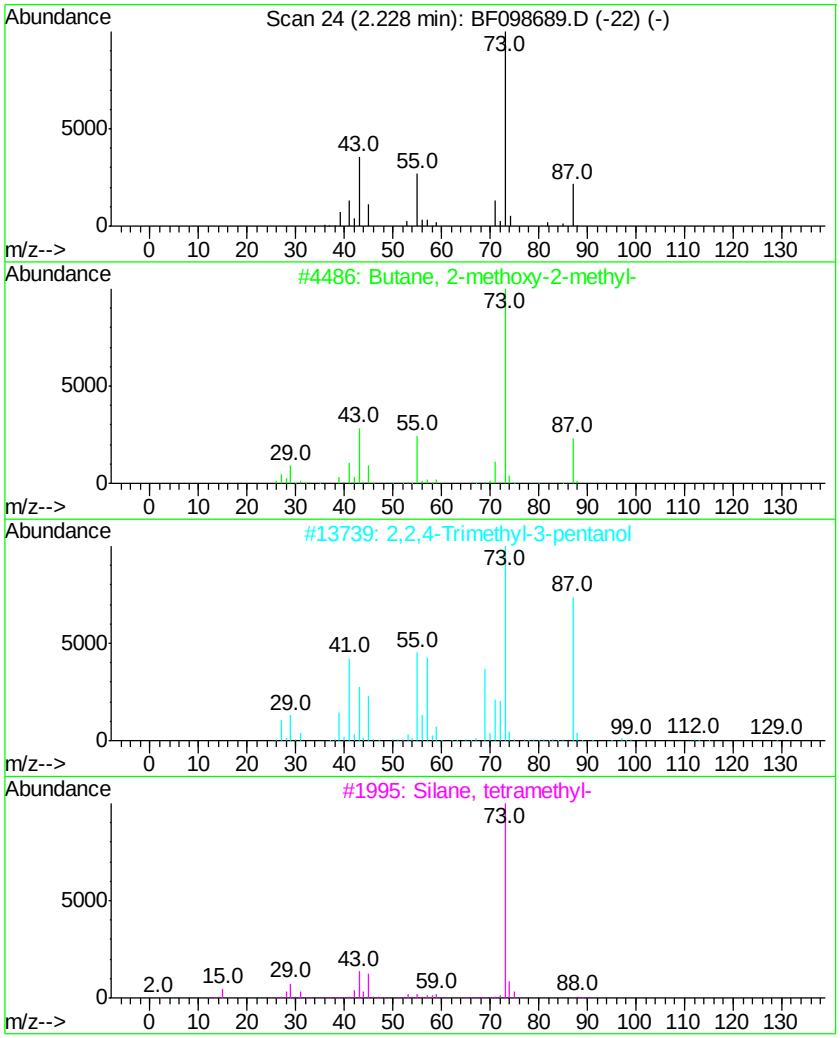
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

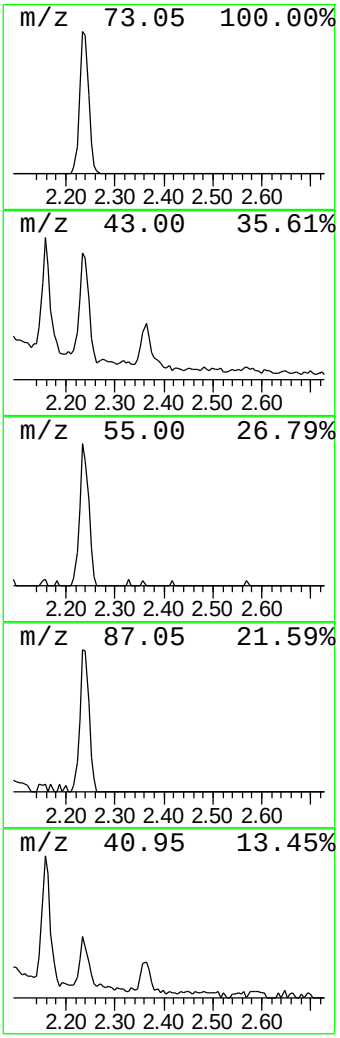
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	4.55 ng	201592	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	25
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	16





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092217\
Data File : BF098689.D
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Operator : SJ/JU
Sample : I5311-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-03-091917

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

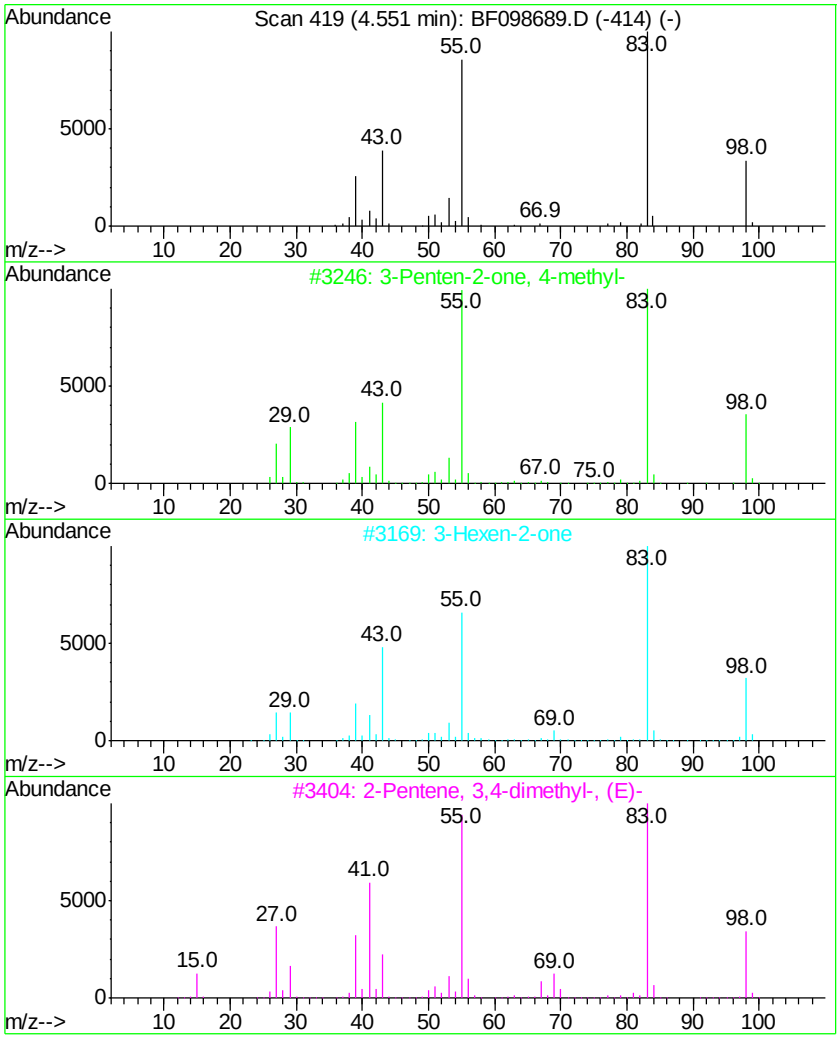
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

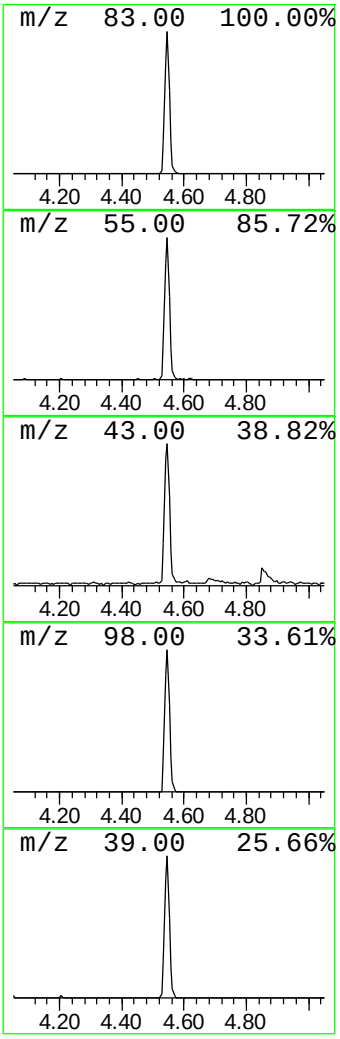
****

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	5.81 ng	257094	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	90
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86





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Sample : I5311-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-03-091917

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

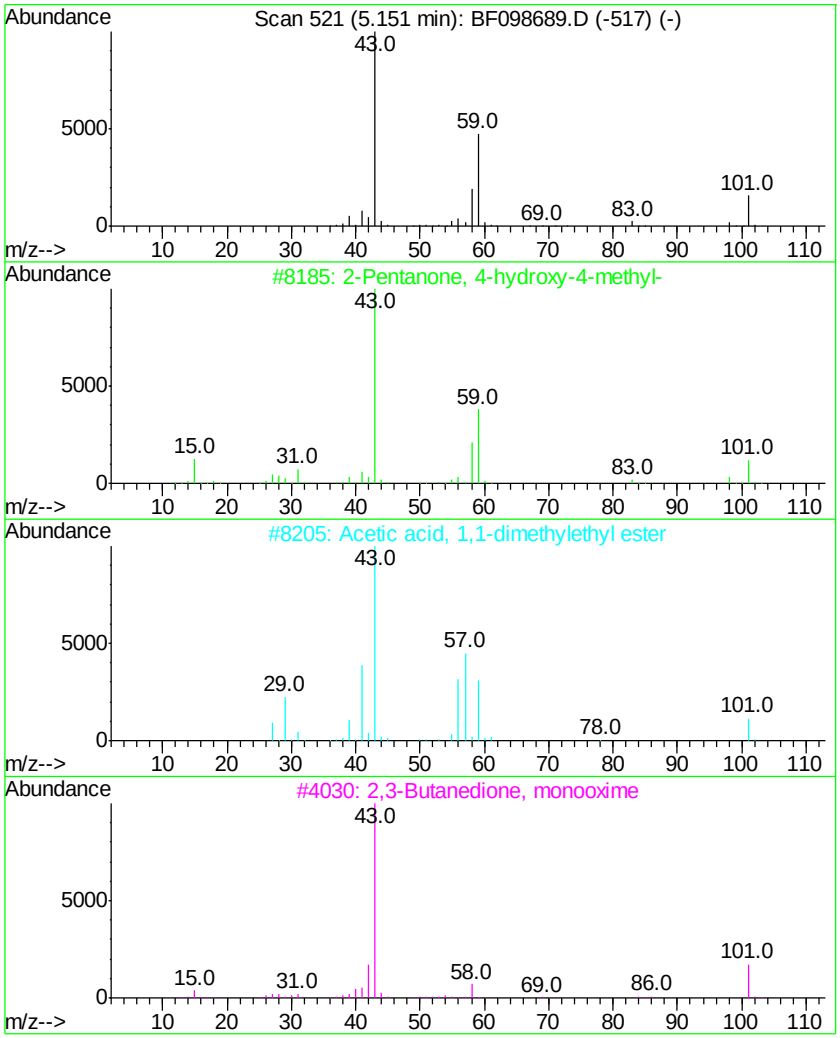
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

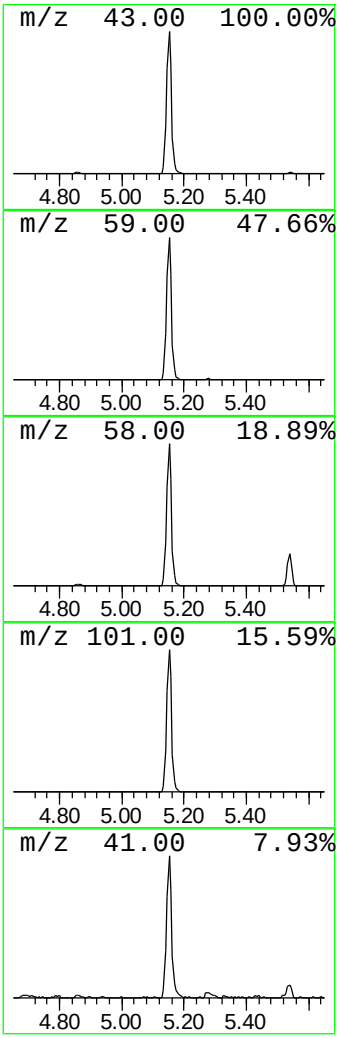
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	21.90 ng	969815	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	78
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Acetone	58	C3H6O	000067-64-1	9





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

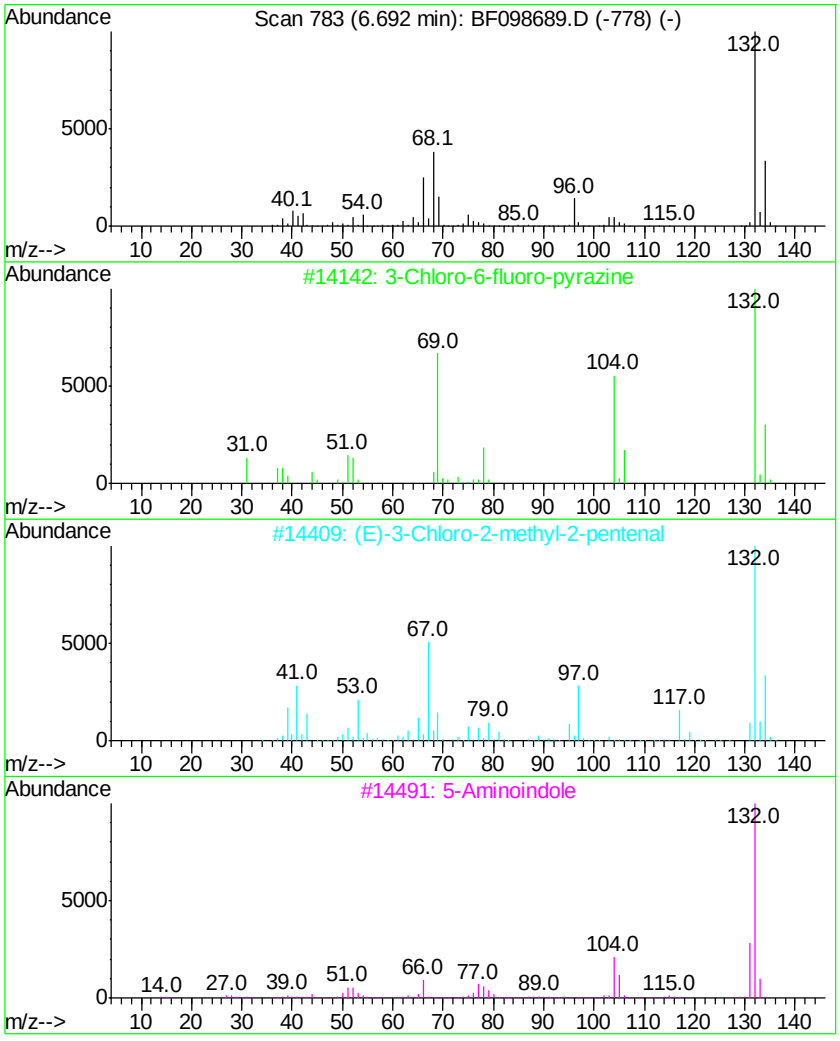
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

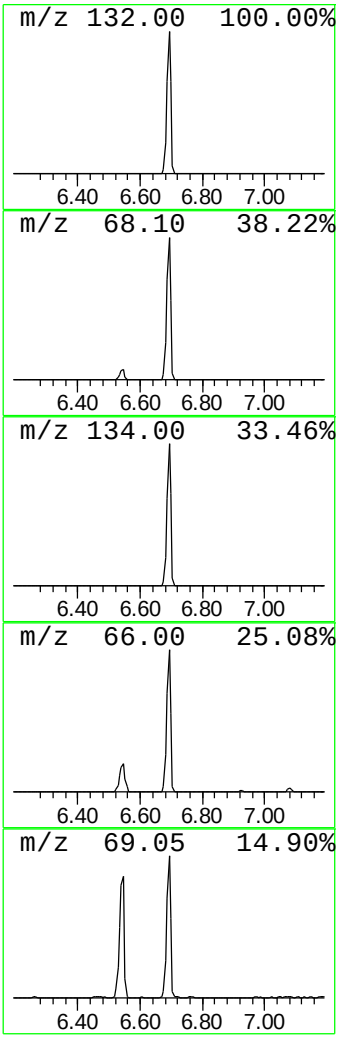
****

Peak Number 5 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	64.18 ng	2842320	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-03-091917

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

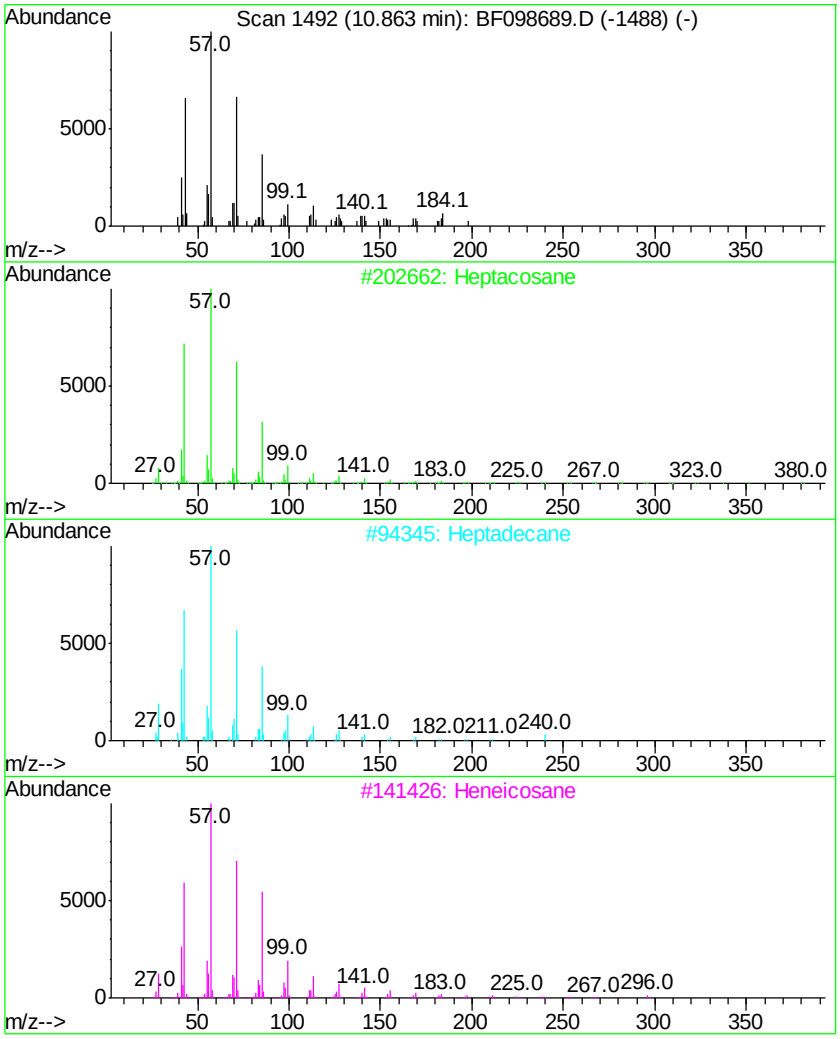
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

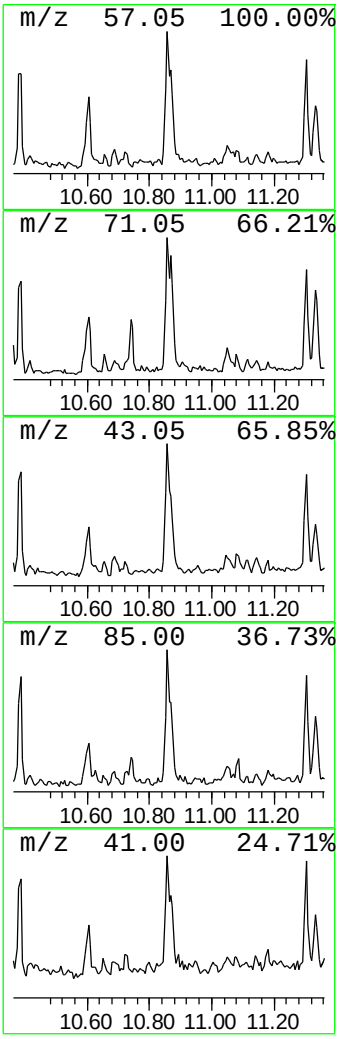
****

Peak Number 7 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.86	3.57 ng	146600	Phenanthrene-d10	11.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Hexadecane	226	C16H34	000544-76-3	90
5	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092217\
Data File : BF098689.D
Acq On : 22 Sep 2017 10:16
Operator : SJ/JU
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-03-091917

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.M
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
3-Penten-2-one	2.16	2.7	ng	118658	1	6.93	885691	20.0
Butane, 2-methoxy...	2.23	4.5	ng	201592	1	6.93	885691	20.0
3-Penten-2-one, 4...	4.55	5.8	ng	257094	1	6.93	885691	20.0
2-Pentanone, 4-hy...	5.15	21.9	ng	969815	1	6.93	885691	20.0
unknown6.69	6.69	64.2	ng	2842320	1	6.93	885691	20.0
Heptacosane	10.86	3.6	ng	146600	4	11.45	820604	20.0