LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071415\
Data File : BF080489.D
Acq On : 15 Jul 2015 13:29
Operator : TP/UM
Sample : G2973-12
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-8D12

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-BF071415.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	2.155	3	6	14	rBV	107716	196860	32.04%	2.671%
2	2.270	14	16	26	rVV	150538	214436	34.90%	2.910%
3	2.430	28	30	34	rVB	4439	7753	1.26%	0.105%
4	4.738	230	232	240	rVB	7274	15660	2.55%	0.212%
5	5.333	281	284	297	rBV	335665	415486	67.61%	5.638%
6	5.756	319	321	333	rBV	550481	536565	87.32%	7.280%
7	6.133	352	354	360	rBV2	34339	38389	6.25%	0.521%
8	6.761	407	409	419	rBV	495994	559635	91.07%	7.594%
9	6.899	419	421	424	rBV	741744	614490	100.00%	8.338%
10	7.127	439	441	443	rBV	138145	169940	27.66%	2.306%
11	7.276	453	454	457	rBV	345596	415047	67.54%	5.632%
12	7.687	488	490	492	rBV	465262	369769	60.17%	5.017%
13	8.407	551	553	556	rBV	278265	241845	39.36%	3.282%
14	9.482	645	647	650	rVB	746063	605637	98.56%	8.218%
15	9.882	679	682	684	rBV	92840	78643	12.80%	1.067%
16	10.168	705	707	710	rBV2	265652	264082	42.98%	3.583%
17	10.568	740	742	747	rVB	8831	8592	1.40%	0.117%
18	10.956	774	776	779	rBV2	280170	334709	54.47%	4.542%
19	11.048	782	784	788	rVB	9146	14221	2.31%	0.193%
20	11.493	821	823	825	rBV	11216	9494	1.55%	0.129%
21	11.665	836	838	842	rVB	336174	323848	52.70%	4.394%
22	11.745	842	845	846	rBV	7179	7119	1.16%	0.097%
23	11.928	857	861	862	rVB2	6446	7311	1.19%	0.099%
24	12.179	881	883	885	rBV	11978	12477	2.03%	0.169%
25	12.305	892	894	897	rVB	7579	9573	1.56%	0.130%
26	12.945	948	950	953	rVB	89735	76474	12.45%	1.038%
27	13.196	968	972	975	rVB	41759	62829	10.22%	0.853%
28	13.345	983	985	988	rBV	482758	545622	88.79%	7.403%
29	13.574	1003	1005	1008	rVB	8258	9496	1.55%	0.129%
30	14.397	1074	1077	1079	rBV	5213	10215	1.66%	0.139%
31	14.442	1079	1081	1087	rVB4	8441	19628	3.19%	0.266%
32	14.625	1094	1097	1099	rBV	303879	358086	58.27%	4.859%
33	14.659	1099	1100	1103	rVB	31286	29439	4.79%	0.399%
34	15.219	1147	1149	1152	rBV	21034	26130	4.25%	0.355%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071415\
Data File : BF080489.D
Acq On : 15 Jul 2015 13:29
Operator : TP/UM
Sample : G2973-12
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-8D12

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-BF071415.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.299	1152	1156	1164	rVB5	6244	20058	3.26%	0.272%
36	15.631	1182	1185	1187	rVB3	3894	7285	1.19%	0.099%
37	15.745	1192	1195	1198	rVV	10233	16352	2.66%	0.222%
38	15.825	1198	1202	1205	rVB3	10399	15280	2.49%	0.207%
39	15.974	1212	1215	1220	rBV	28910	69166	11.26%	0.938%
40	16.054	1220	1222	1225	rVB	44860	52758	8.59%	0.716%
41	16.145	1228	1230	1233	rBV3	3746	7853	1.28%	0.107%
42	16.328	1244	1246	1250	rVB	16850	20642	3.36%	0.280%
43	16.397	1250	1252	1255	rVB	24304	31742	5.17%	0.431%
44	16.477	1255	1259	1266	rBV	199614	332654	54.13%	4.514%
45	16.717	1277	1280	1284	rVB5	4946	12612	2.05%	0.171%
46	16.968	1299	1302	1306	rVB	16959	27895	4.54%	0.378%
47	17.848	1376	1379	1384	rBV3	3997	8689	1.41%	0.118%
48	18.134	1401	1404	1409	rBV3	11146	28480	4.63%	0.386%
49	18.626	1444	1447	1452	rVB	8668	15910	2.59%	0.216%
50	18.843	1459	1466	1478	rVB	15215	93045	15.14%	1.262%

Sum of corrected areas: 7369921

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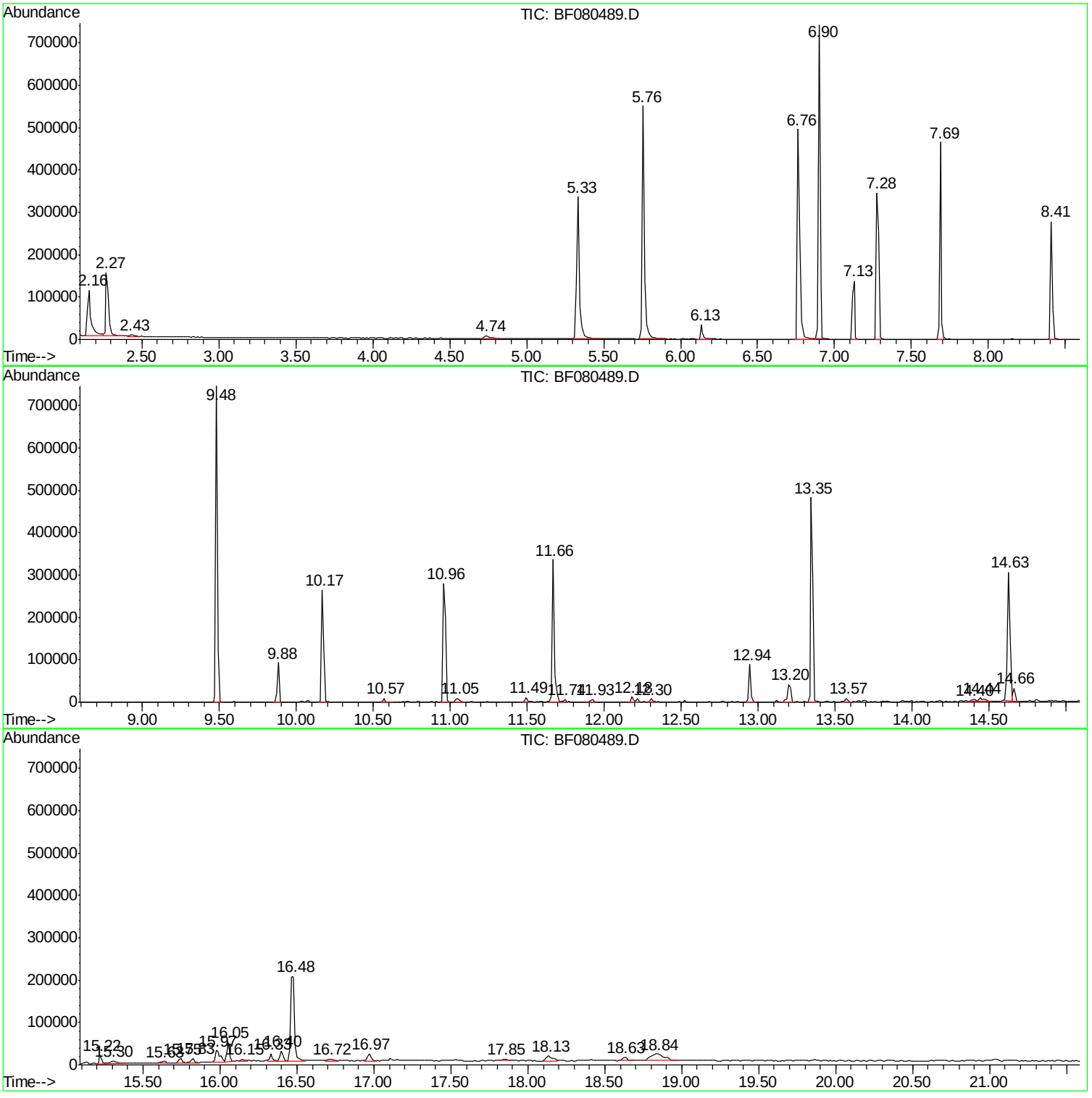
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-8D12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071415\
Data File : BF080489.D
Acq On : 15 Jul 2015 13:29
Operator : TP/UM
Sample : G2973-12
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-8D12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

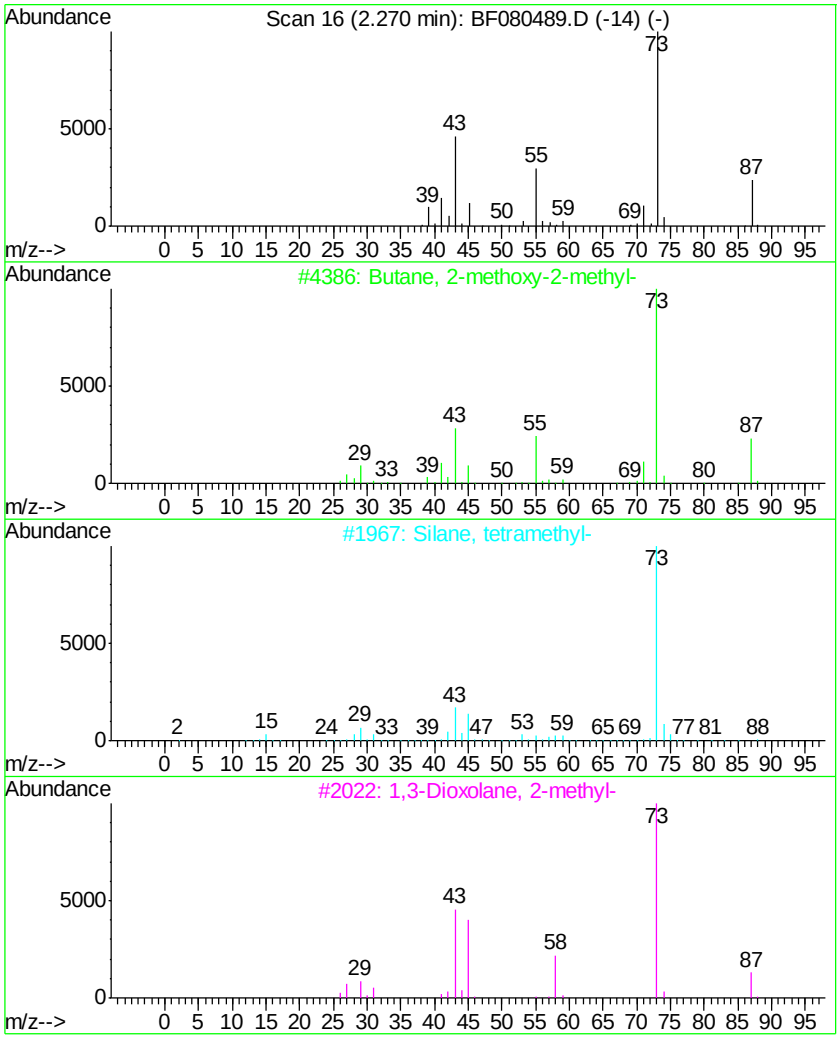
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

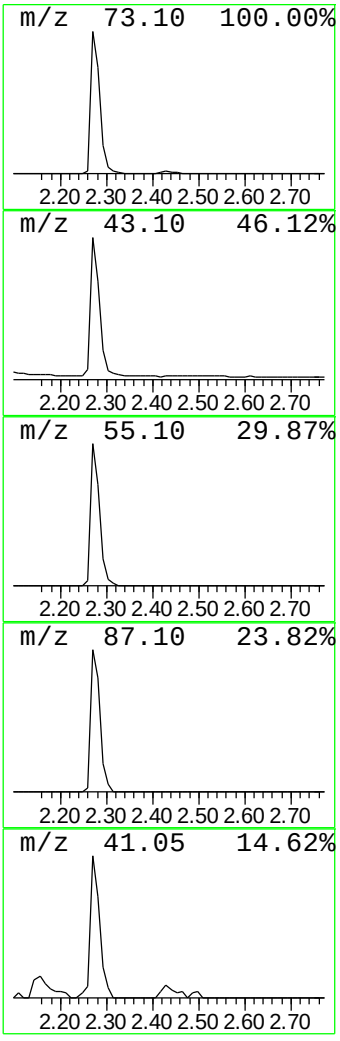
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.27	25.24 ng	214436	1,4-Dichlorobenzene-d4	7.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071415\
Data File : BF080489.D
Acq On : 15 Jul 2015 13:29
Operator : TP/UM
Sample : G2973-12
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-8D12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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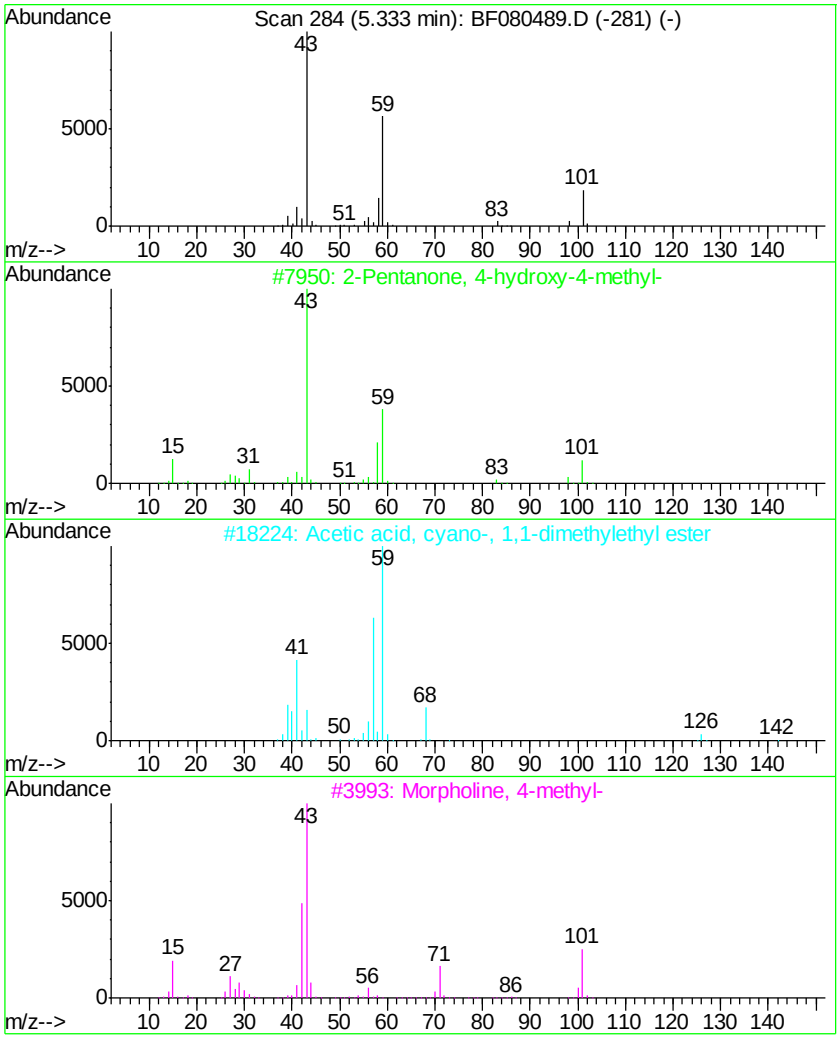
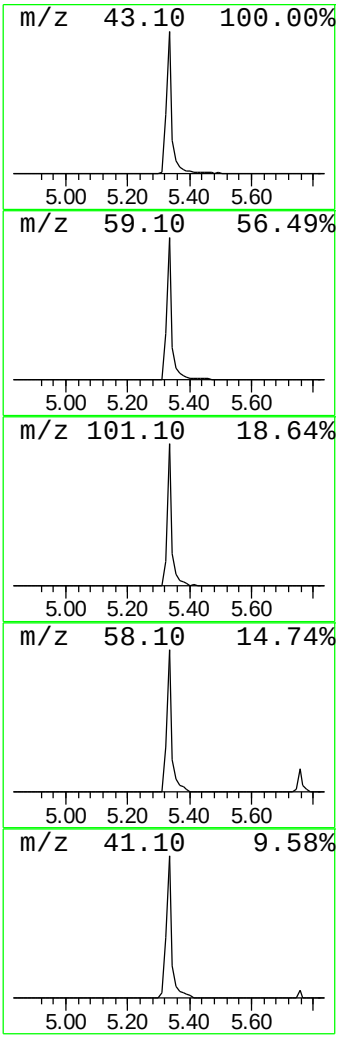
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	48.90 ng	415486	1,4-Dichlorobenzene-d4	7.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071415\
Data File : BF080489.D
Acq On : 15 Jul 2015 13:29
Operator : TP/UM
Sample : G2973-12
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-8D12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

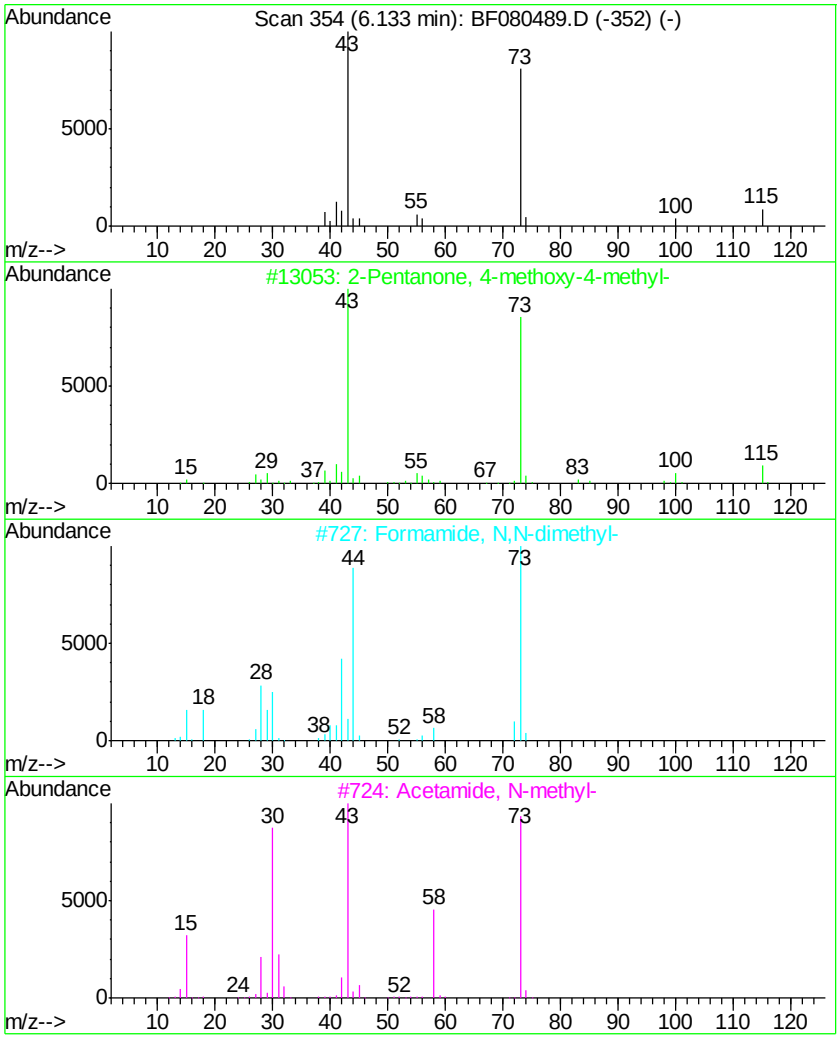
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

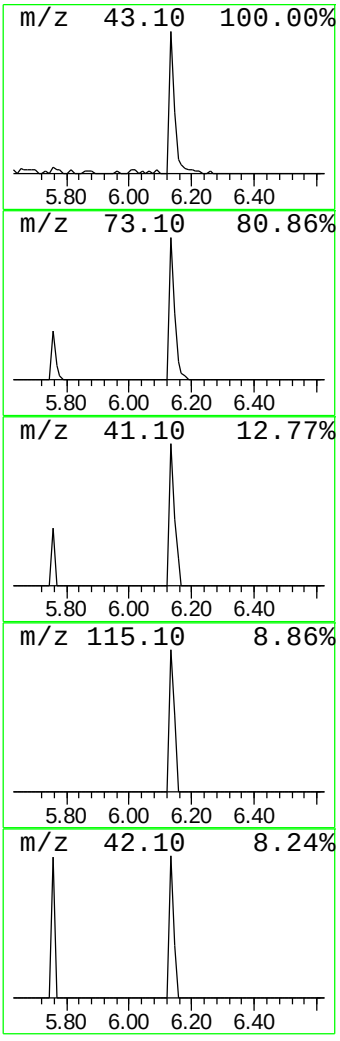
****

Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.13	4.52 ng	38389	1,4-Dichlorobenzene-d4	7.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	Formamide, N,N-dimethyl-	73	C3H7NO	000068-12-2	9
3	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
4	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	9
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071415\
Data File : BF080489.D
Acq On : 15 Jul 2015 13:29
Operator : TP/UM
Sample : G2973-12
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-8D12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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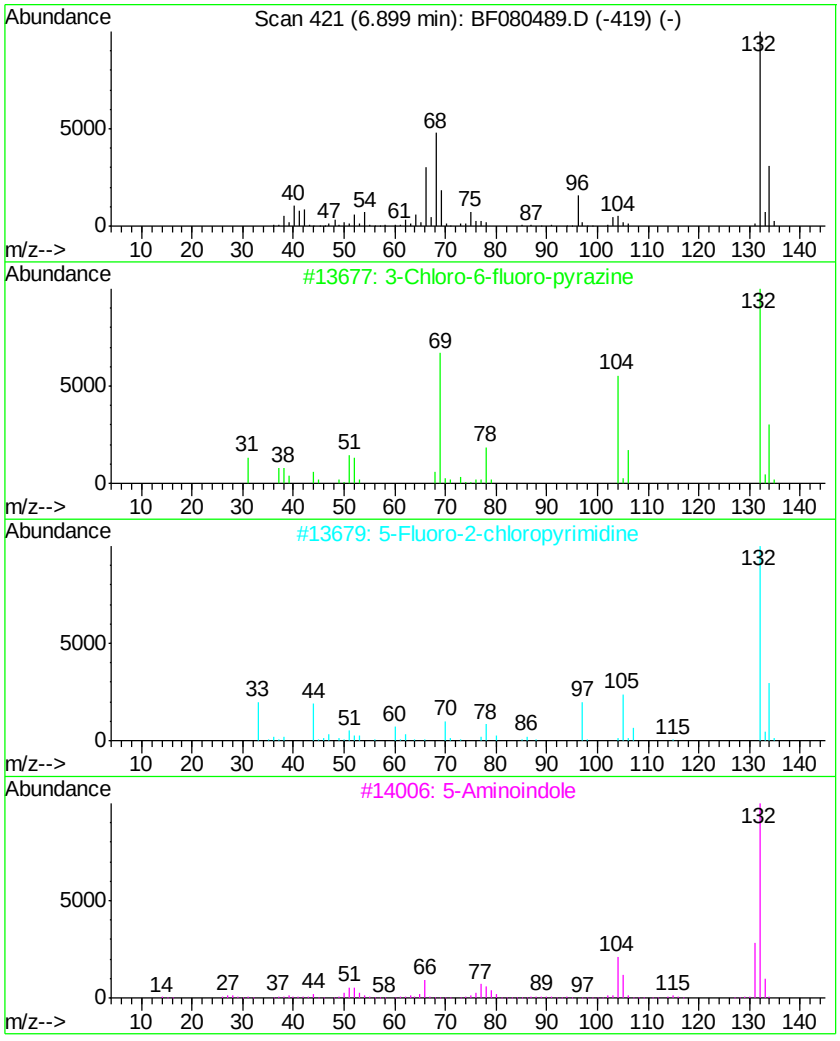
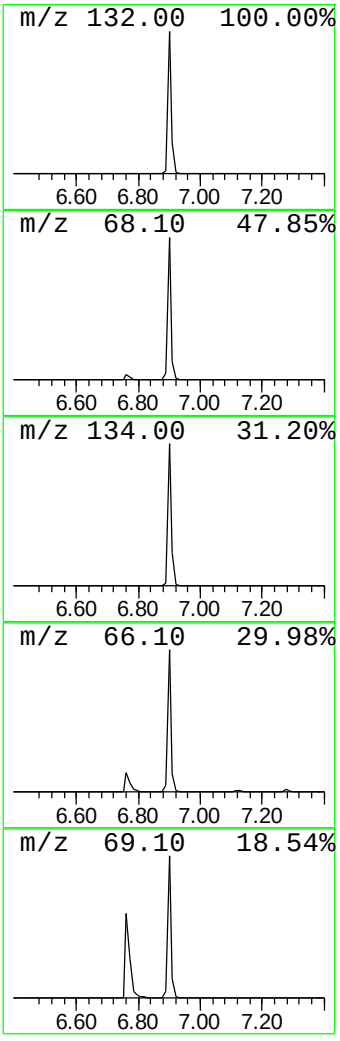
Peak Number 5 unknown6.90 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.90	72.32 ng	614490	1,4-Dichlorobenzene-d4	7.13

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	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Acq On : 15 Jul 2015 13:29
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Sample : G2973-12
Misc :
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Instrument : BNA_F
ClientSampleId : TP-8D12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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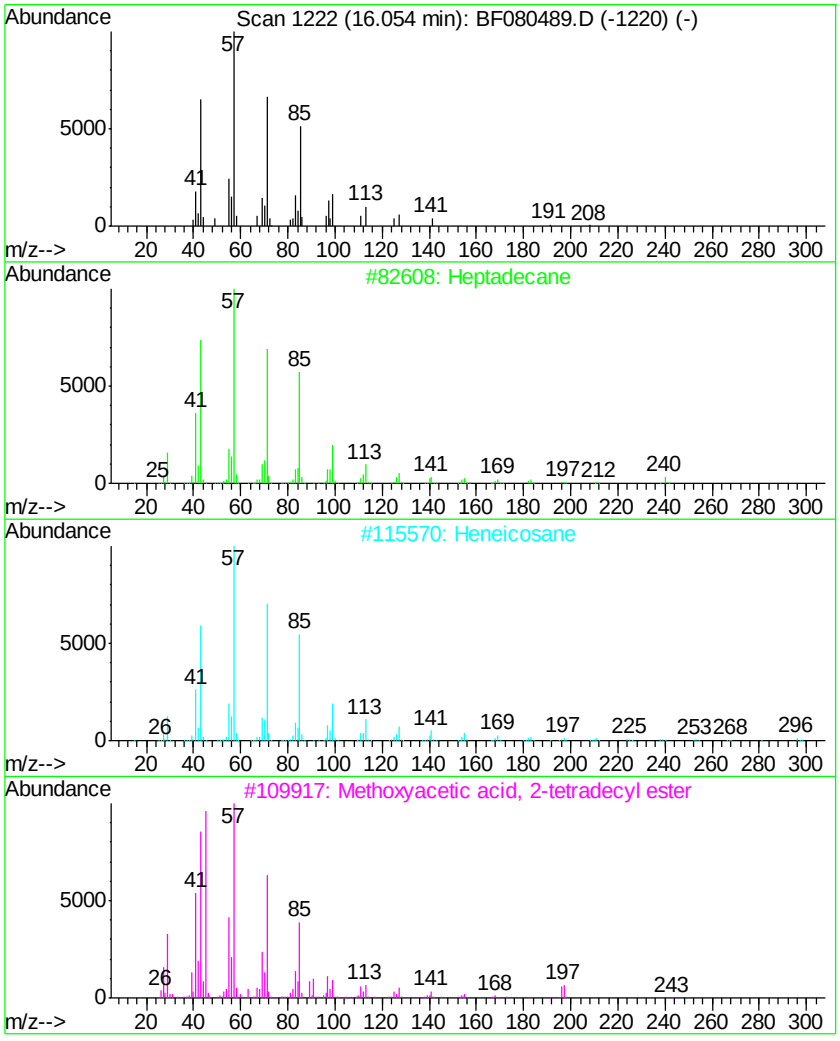
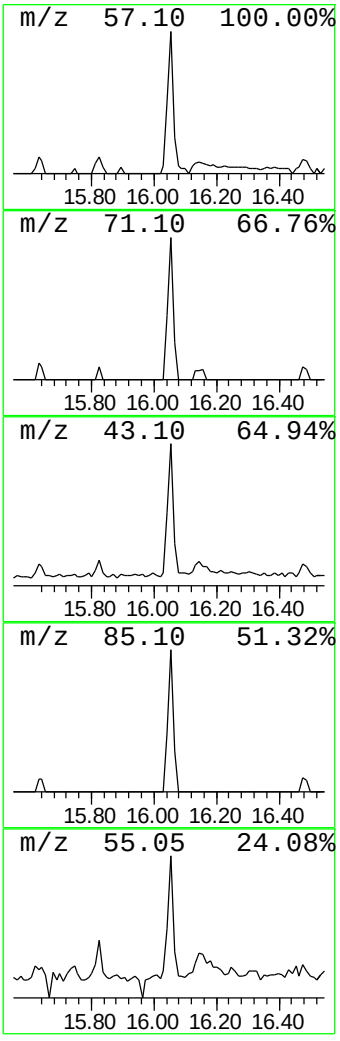
Peak Number 8 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.05	3.17 ng	52758	Perylene-d12	16.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	87
2	Heneicosane	296	C21H44	000629-94-7	87
3	Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	86
4	Hexatriacontane	507	C36H74	000630-06-8	86
5	Tetracosane	338	C24H50	000646-31-1	86





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Acq On : 15 Jul 2015 13:29
Operator : TP/UM
Sample : G2973-12
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-8D12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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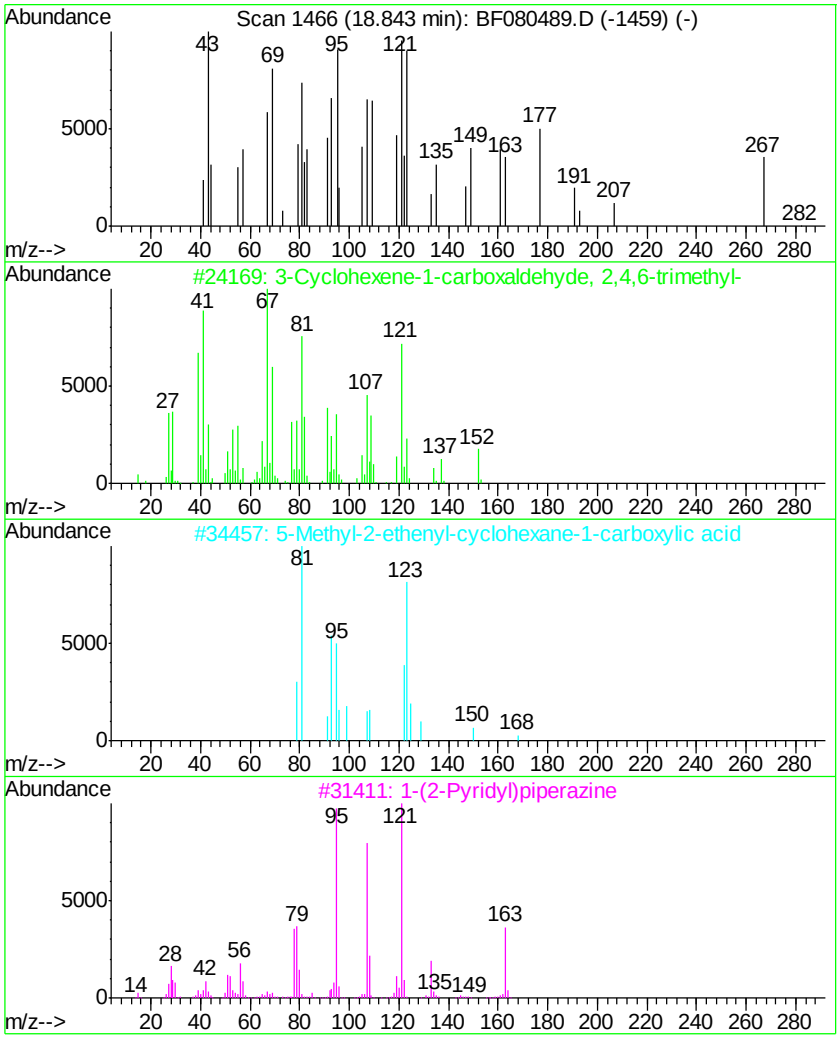
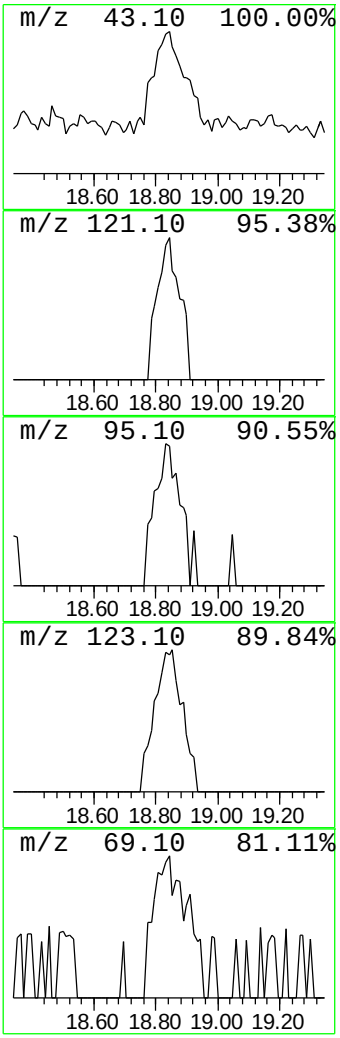
Peak Number 9 unknown18.84 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.84	5.59 ng	93045	Perylene-d12	16.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	001423-46-7	43
2	5-Methyl-2-ethenyl-cyclohexane-1...	168	C10H16O2	1000144-53-6	27
3	1-(2-Pyridyl)piperazine	163	C9H13N3	034803-66-2	25
4	(-)-Neoclovene-(II), dihydro-	206	C15H26	1000152-83-6	22
5	(-)-Neoclovene-(I), dihydro-	206	C15H26	1000152-82-1	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071415\
Data File : BF080489.D
Acq On : 15 Jul 2015 13:29
Operator : TP/UM
Sample : G2973-12
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-8D12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.27	25.2	ng	214436	1	7.13	169940	20.0
2-Pentanone, 4-hy...	5.33	48.9	ng	415486	1	7.13	169940	20.0
2-Pentanone, 4-me...	6.13	4.5	ng	38389	1	7.13	169940	20.0
unknown6.90	6.90	72.3	ng	614490	1	7.13	169940	20.0
Heptadecane	16.05	3.2	ng	52758	6	16.48	332654	20.0
unknown18.84	18.84	5.6	ng	93045	6	16.48	332654	20.0