LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100317\
Data File : BF099056.D
Acq On : 4 Oct 2017 3:16
Operator : SJ/JU
Sample : I5486-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PAMT-SSW

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-BF092317.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	2.163	9	13	27	rVB	467785	658931	22.44%	2.740%
2	2.998	151	155	161	rVB	18716	31348	1.07%	0.130%
3	3.616	256	260	268	rBV	77050	114611	3.90%	0.477%
4	4.481	402	407	421	rVB	1195928	1316304	44.83%	5.473%
5	4.739	446	451	457	rBV	53775	57978	1.97%	0.241%
6	5.098	509	512	523	rVB	60864	69453	2.37%	0.289%
7	5.492	575	579	587	rBV	1844884	1642346	55.94%	6.828%
8	6.498	745	750	760	rVB	1002261	923800	31.46%	3.841%
9	6.645	770	775	778	rBV	3007599	2713004	92.40%	11.280%
10	6.875	810	814	817	rBV	1048126	820723	27.95%	3.412%
11	7.033	836	841	844	rBV	2779620	2537846	86.44%	10.551%
12	7.439	904	910	913	rBV	2025043	1938087	66.01%	8.058%
13	8.157	1028	1032	1035	rBV	1047164	955021	32.53%	3.971%
14	9.227	1209	1214	1217	rBV	3111204	2936059	100.00%	12.207%
15	9.616	1277	1280	1283	rBV	114379	95019	3.24%	0.395%
16	9.910	1326	1330	1334	rVB	832569	688011	23.43%	2.860%
17	10.574	1440	1443	1446	rVB	284714	205378	7.00%	0.854%
18	10.698	1460	1464	1472	rVB	1467579	1329889	45.30%	5.529%
19	10.804	1478	1482	1492	rBV	29571	32616	1.11%	0.136%
20	11.392	1579	1582	1586	rBV	739624	669729	22.81%	2.784%
21	12.792	1814	1820	1823	rBV	44089	36853	1.26%	0.153%
22	12.868	1830	1833	1836	rVB	46817	38998	1.33%	0.162%
23	12.980	1847	1852	1855	rBV	2655894	2364011	80.52%	9.829%
24	13.868	1999	2003	2005	rBV	30187	32262	1.10%	0.134%
25	14.033	2027	2031	2035	rBV	950142	788360	26.85%	3.278%
26	14.486	2105	2108	2112	rBV4	32231	38290	1.30%	0.159%
27	14.798	2157	2161	2164	rBV	28524	36676	1.25%	0.152%
28	15.133	2213	2218	2221	rBV4	29086	41475	1.41%	0.172%
29	15.509	2277	2282	2293	rBV2	458600	636751	21.69%	2.647%
30	15.956	2354	2358	2362	rVB	32395	48499	1.65%	0.202%
31	16.127	2384	2387	2392	rVB6	20726	29753	1.01%	0.124%
32	16.233	2402	2405	2413	rVB6	55263	85672	2.92%	0.356%
33	16.462	2440	2444	2450	rVB2	28143	46253	1.58%	0.192%
34	17.056	2542	2545	2554	rVB5	21333	41508	1.41%	0.173%

LSC Area Percent Report

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Instrument : BNA_F
ClientSampleId : PAMT-SSW

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Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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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-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.762	2659	2665	2672	rBV8	19708	50630	1.72%	0.211%	

Sum of corrected areas: 24052144

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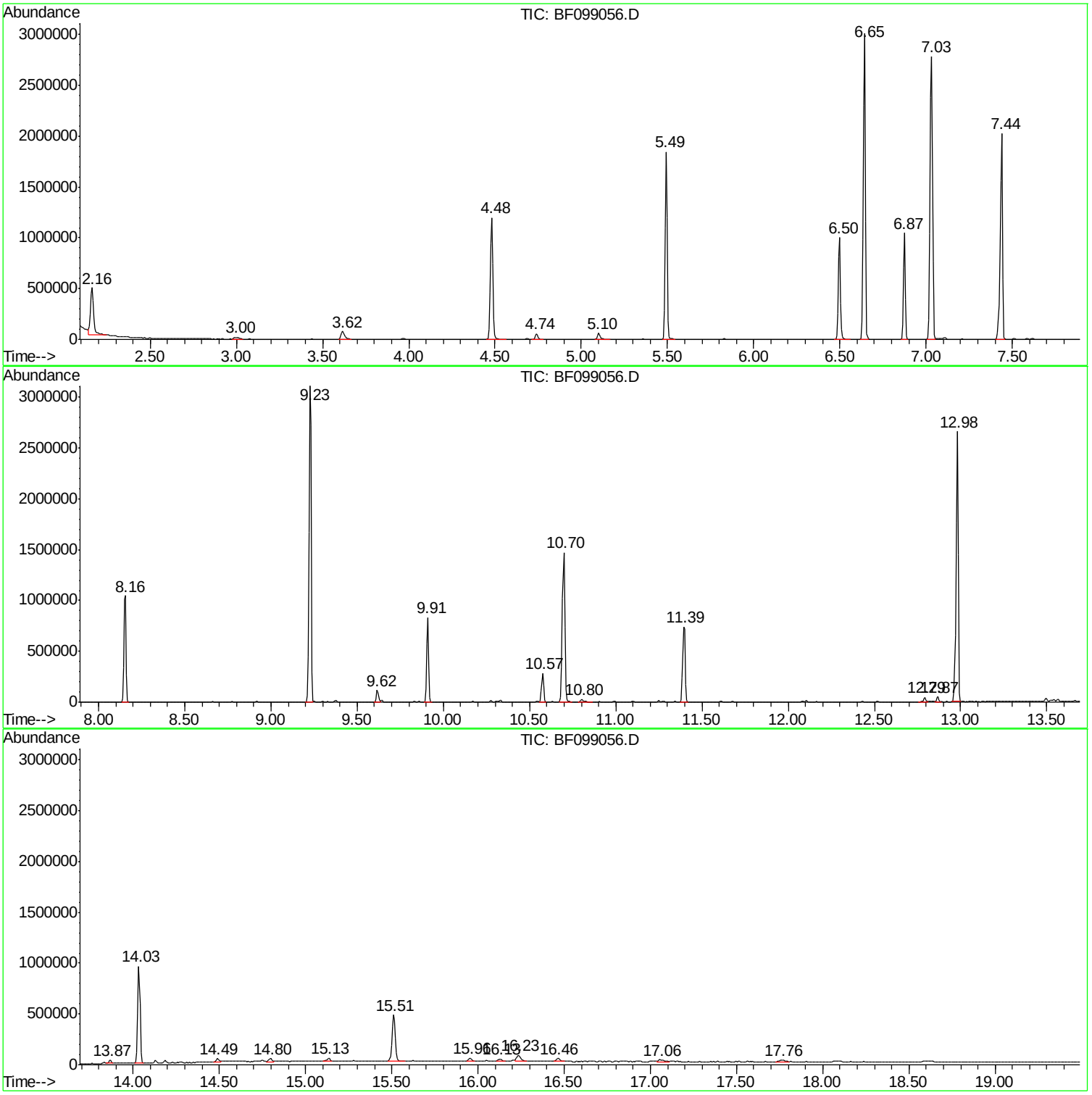
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PAMT-SSW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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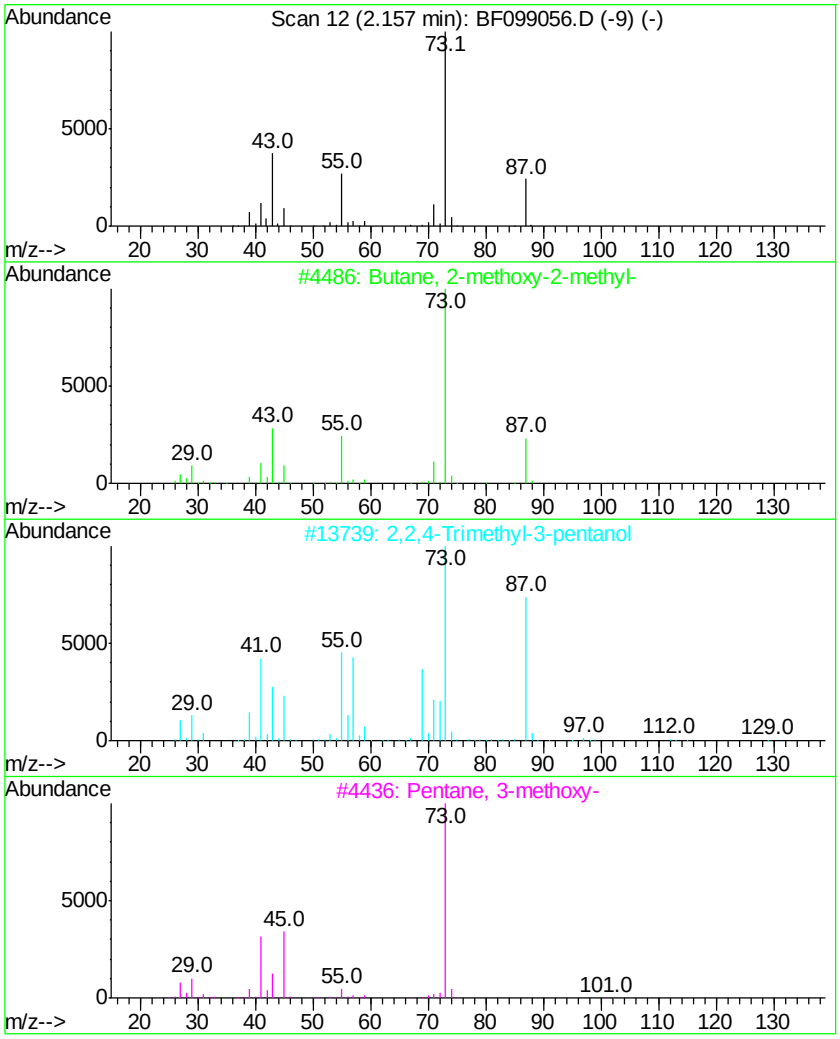
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

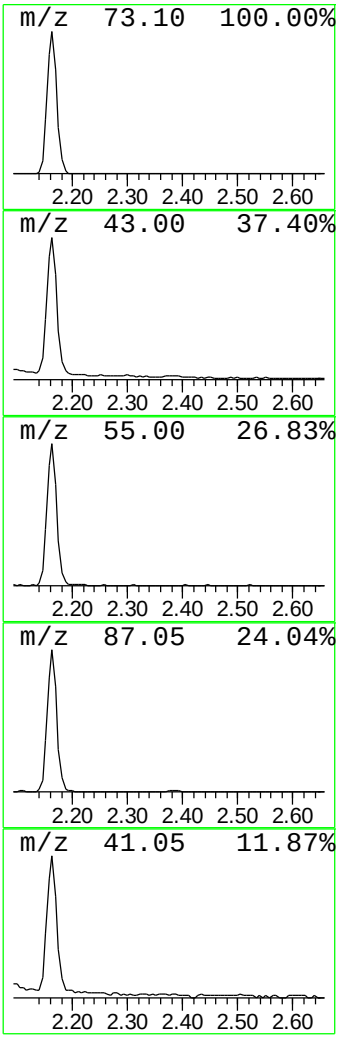
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	16.06 ng	658931	1,4-Dichlorobenzene-d4	6.87

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	40
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100317\
Data File : BF099056.D
Acq On : 4 Oct 2017 3:16
Operator : SJ/JU
Sample : I5486-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PAMT-SSW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

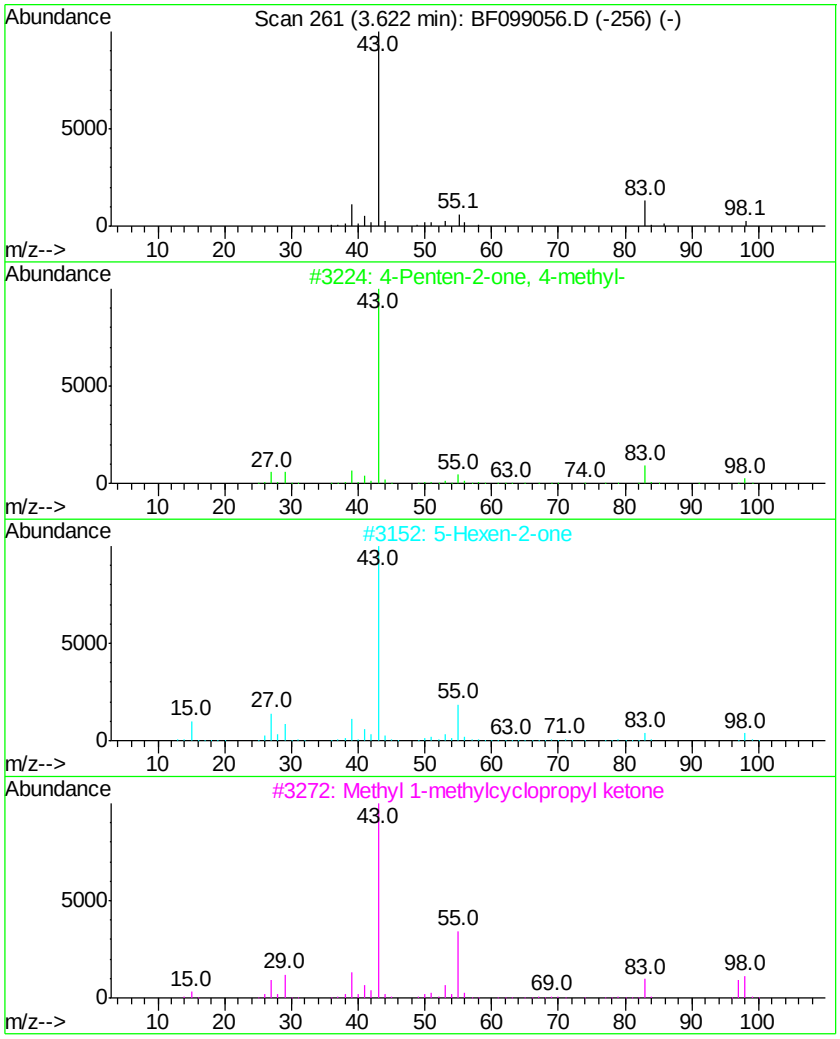
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

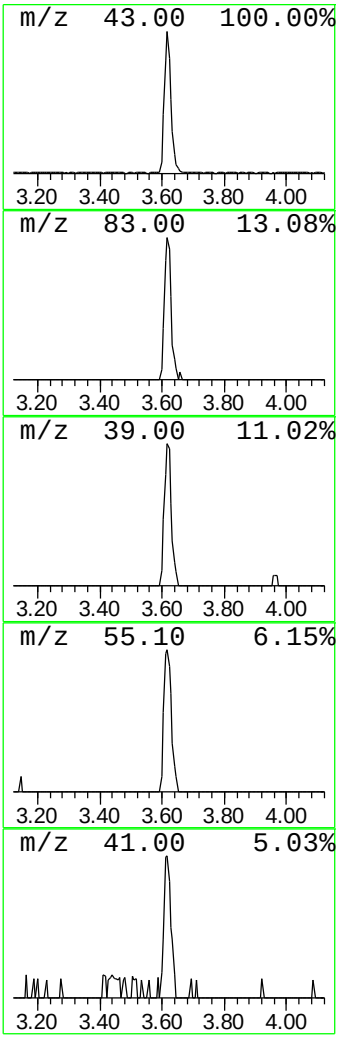
****

Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.62	2.79 ng	114611	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	64
2	5-Hexen-2-one	98	C6H10O	000109-49-9	16
3	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	9
4	4-Hexen-2-one	98	C6H10O	025659-22-7	9
5	2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	9





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Operator : SJ/JU
Sample : I5486-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PAMT-SSW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

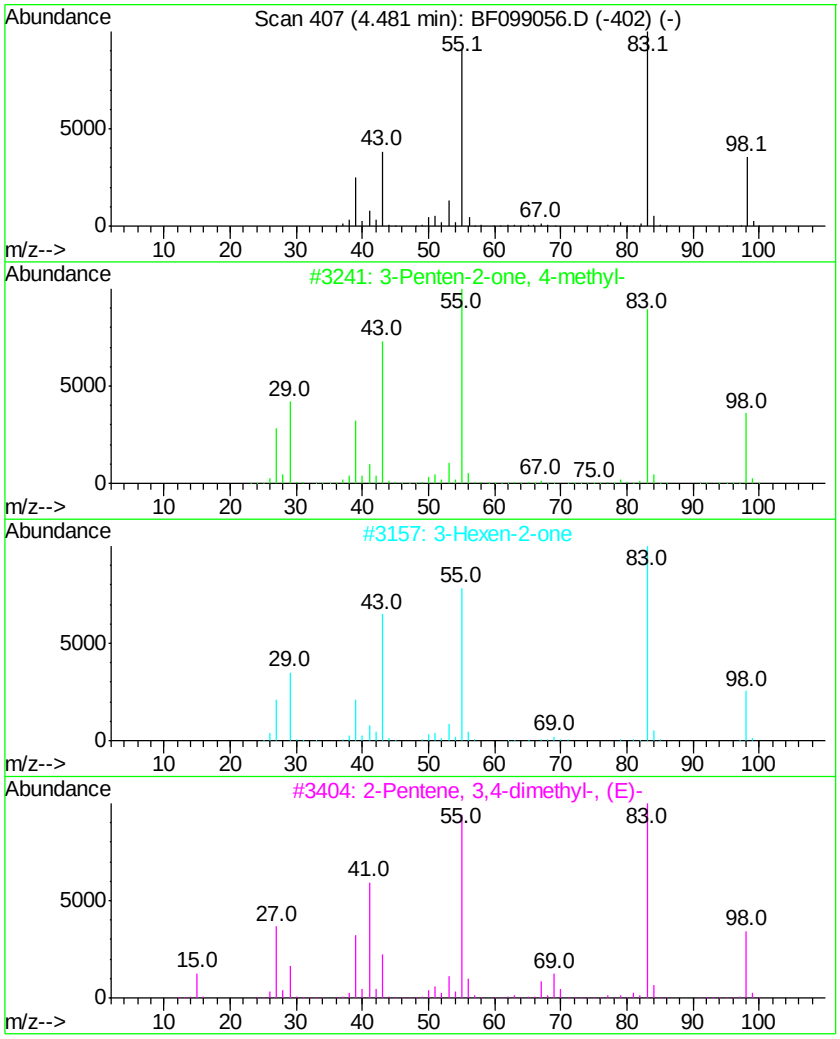
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

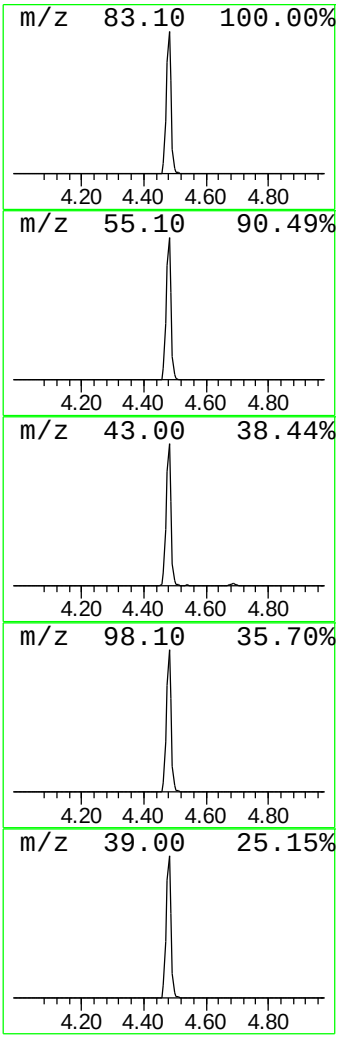
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.48	32.08 ng	1316300	1,4-Dichlorobenzene-d4	6.87

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	91
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	80





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Operator : SJ/JU
Sample : I5486-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PAMT-SSW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

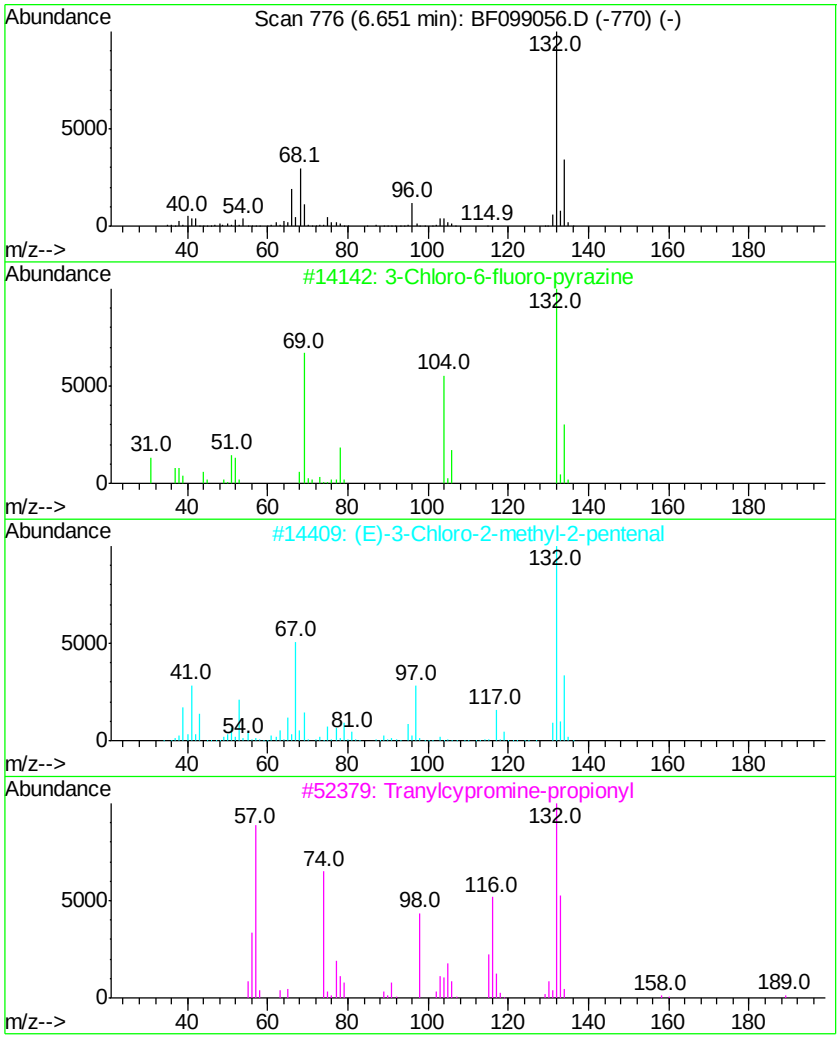
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

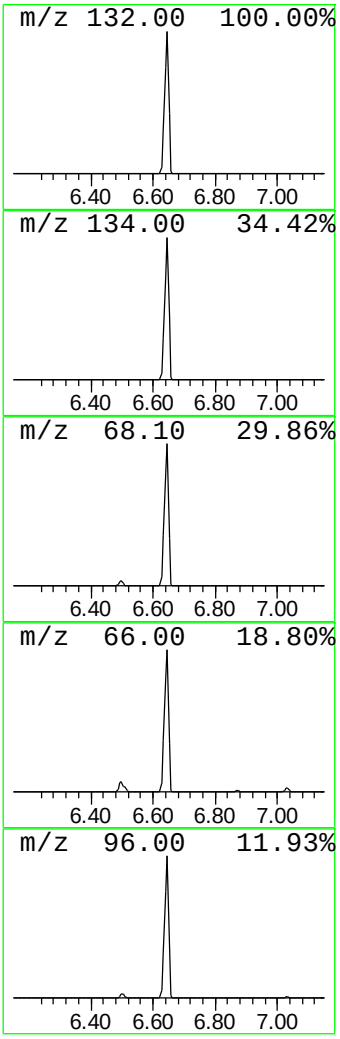
****

Peak Number 4 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	66.11 ng	2713000	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

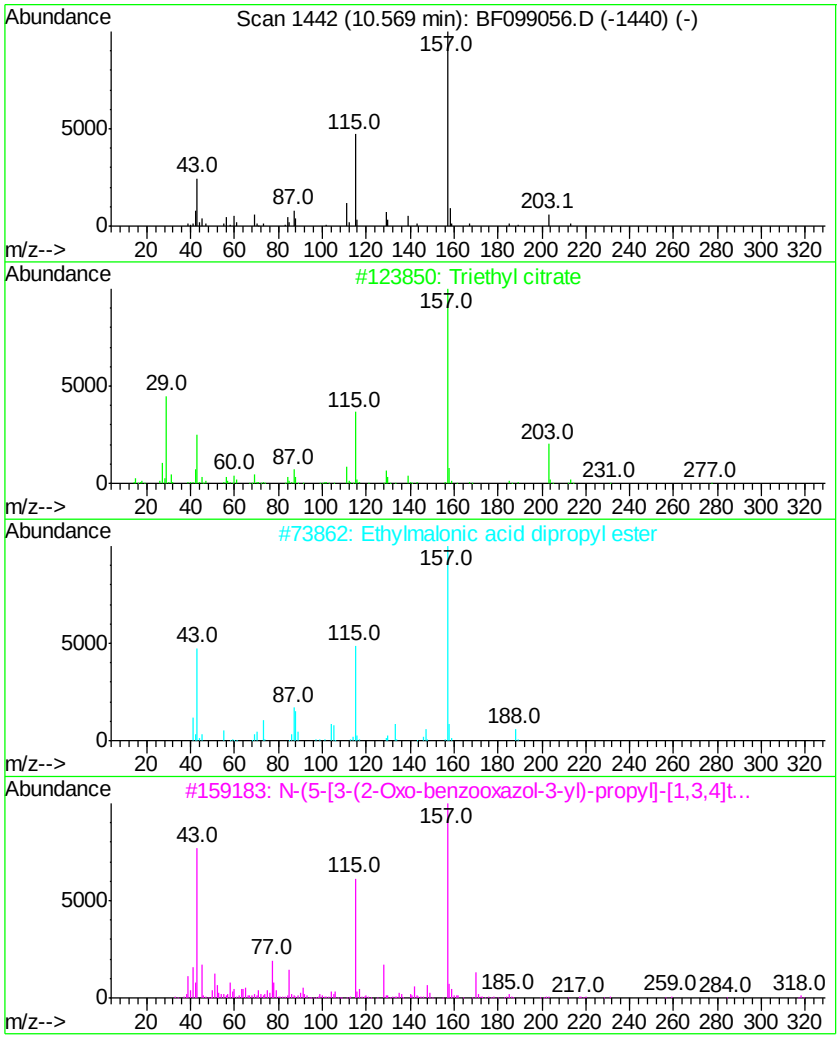
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

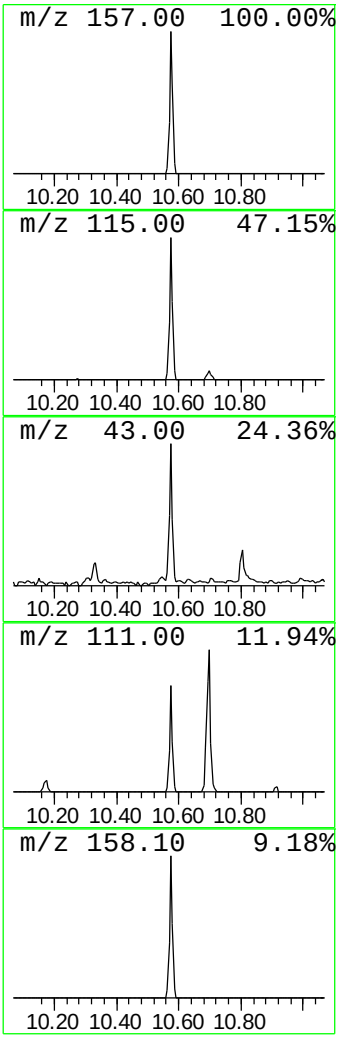
****

Peak Number 6 Triethyl citrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.57	5.97 ng	205378	Acenaphthene-d10	9.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	91
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	50
3	N-(5-[3-(2-Oxo-benzooxazol-3-yl)...	318	C14H14N4O3S	1000300-11-5	38
4	Adipic acid, ethyl pent-4-en-2-y...	242	C13H22O4	1000354-11-7	37
5	Octanedioic acid, bis(1-methylpr...	286	C16H30O4	057983-35-4	33





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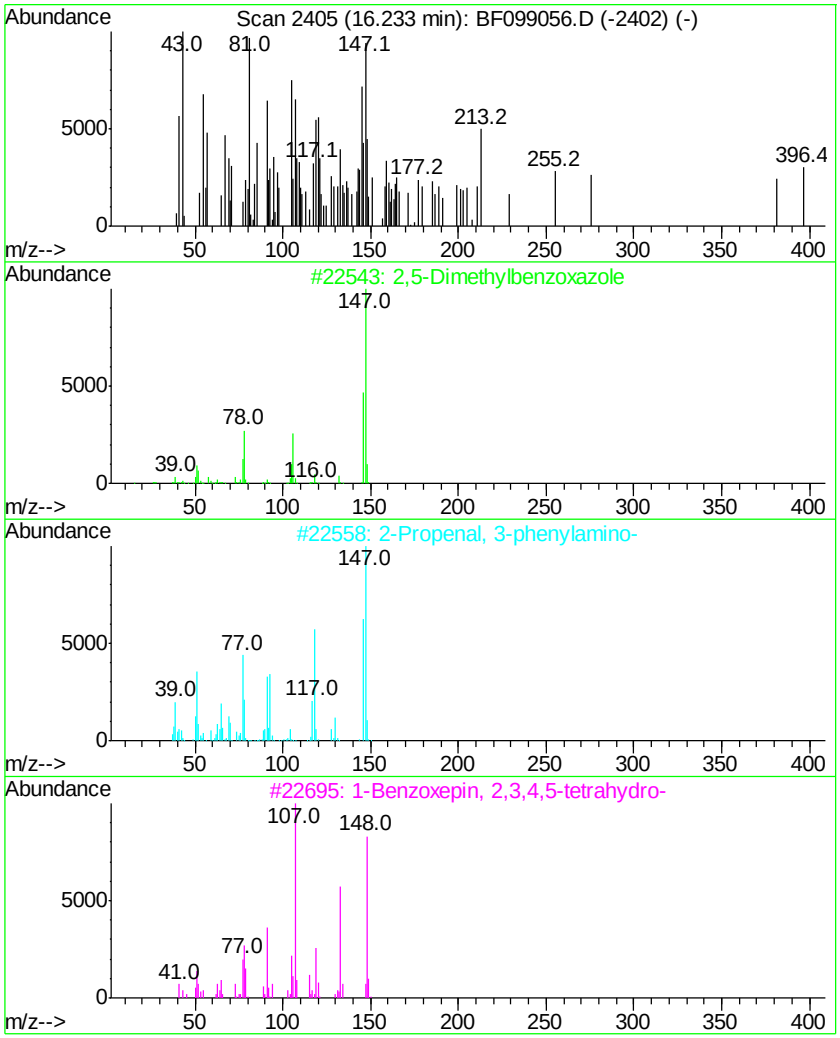
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

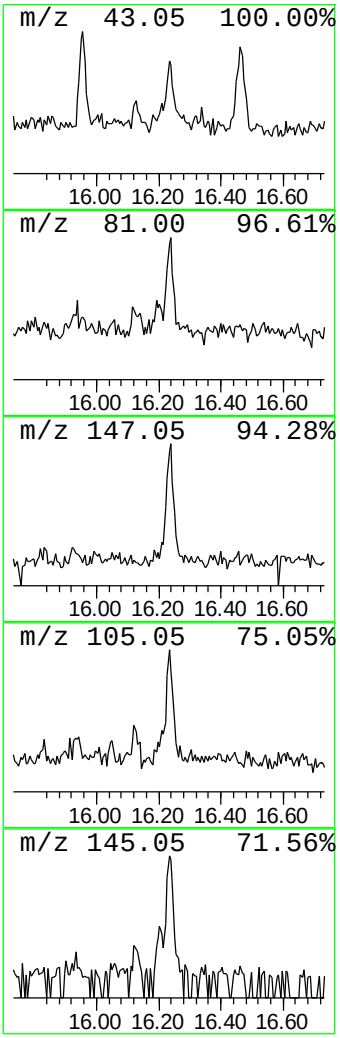
****

Peak Number 7 unknown16.23 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.23	2.69 ng	85672	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Dimethylbenzoxazole	147	C9H9NO	005676-58-4	22
2	2-Propenal, 3-phenylamino-	147	C9H9NO	025299-39-2	14
3	1-Benzoxepin, 2,3,4,5-tetrahydro-	148	C10H12O	006169-78-4	11
4	6-Methyl-1,2,3,5,8,8a-hexahydron...	148	C11H16	107914-86-3	11
5	2(3H)-Benzofuranone, 3-methyl-	148	C9H8O2	032267-71-3	11





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
Butane, 2-methoxy...	2.16	16.1	ng	658931	1	6.87	820723	20.0
4-Penten-2-one, 4...	3.62	2.8	ng	114611	1	6.87	820723	20.0
3-Penten-2-one, 4...	4.48	32.1	ng	1316300	1	6.87	820723	20.0
unknown6.65	6.65	66.1	ng	2713000	1	6.87	820723	20.0
Triethyl citrate	10.57	6.0	ng	205378	3	9.91	688011	20.0
unknown16.23	16.23	2.7	ng	85672	6	15.51	636751	20.0