LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100917\
Data File : BF099275.D
Acq On : 9 Oct 2017 21:13
Operator : SJ/JU
Sample : I5715-13 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-02-100517-E

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	5.069	505	507	520	rBB	54883	60018	7.41%	0.797%
2	5.475	573	576	592	rBV	418291	371671	45.89%	4.937%
3	6.487	745	748	758	rBV	427850	375595	46.37%	4.989%
4	6.628	769	772	776	rBV	506648	415440	51.29%	5.518%
5	6.863	808	812	816	rBV	714259	581853	71.84%	7.729%
6	7.016	835	838	842	rBV	405551	316434	39.07%	4.203%
7	7.422	904	907	915	rBV	290316	229180	28.30%	3.044%
8	8.145	1026	1030	1033	rBV	992321	778049	96.06%	10.335%
9	8.410	1072	1075	1078	rBB	16560	11535	1.42%	0.153%
10	9.216	1208	1212	1223	rBV	609128	479105	59.15%	6.364%
11	9.610	1276	1279	1286	rBV	61896	51620	6.37%	0.686%
12	9.822	1310	1315	1318	rBV	59763	52469	6.48%	0.697%
13	9.898	1324	1328	1336	rVB	936522	809945	100.00%	10.759%
14	10.316	1395	1399	1402	rVB2	9702	13274	1.64%	0.176%
15	10.686	1459	1462	1467	rBV	225539	190230	23.49%	2.527%
16	10.792	1477	1480	1485	rBV2	11002	12218	1.51%	0.162%
17	11.386	1577	1581	1584	rBV	847107	702842	86.78%	9.336%
18	11.969	1677	1680	1683	rBV2	14837	16041	1.98%	0.213%
19	11.998	1683	1685	1688	rBV3	16869	23843	2.94%	0.317%
20	12.180	1712	1716	1721	rBV2	26104	34723	4.29%	0.461%
21	12.474	1761	1766	1768	rVV4	25759	27895	3.44%	0.371%
22	12.522	1771	1774	1778	rBV5	6200	9806	1.21%	0.130%
23	12.598	1784	1787	1790	rBV	51932	46084	5.69%	0.612%
24	12.757	1808	1814	1815	rBV4	7689	11514	1.42%	0.153%
25	12.827	1821	1826	1830	rBV	52857	58742	7.25%	0.780%
26	12.963	1846	1849	1853	rBV	394734	339503	41.92%	4.510%
27	13.104	1871	1873	1875	rBV2	12988	12916	1.59%	0.172%
28	13.133	1875	1878	1880	rVV4	11444	13872	1.71%	0.184%
29	13.404	1922	1924	1929	rVB6	14536	15380	1.90%	0.204%
30	14.027	2026	2030	2033	rBV	641278	577487	71.30%	7.671%
31	15.504	2277	2281	2287	rVB2	444546	553647	68.36%	7.354%
32	16.192	2395	2398	2407	rVB2	102845	184539	22.78%	2.451%
33	16.633	2469	2473	2478	rVB	95687	150745	18.61%	2.002%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
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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

Sum of corrected areas: 7528215

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100917\
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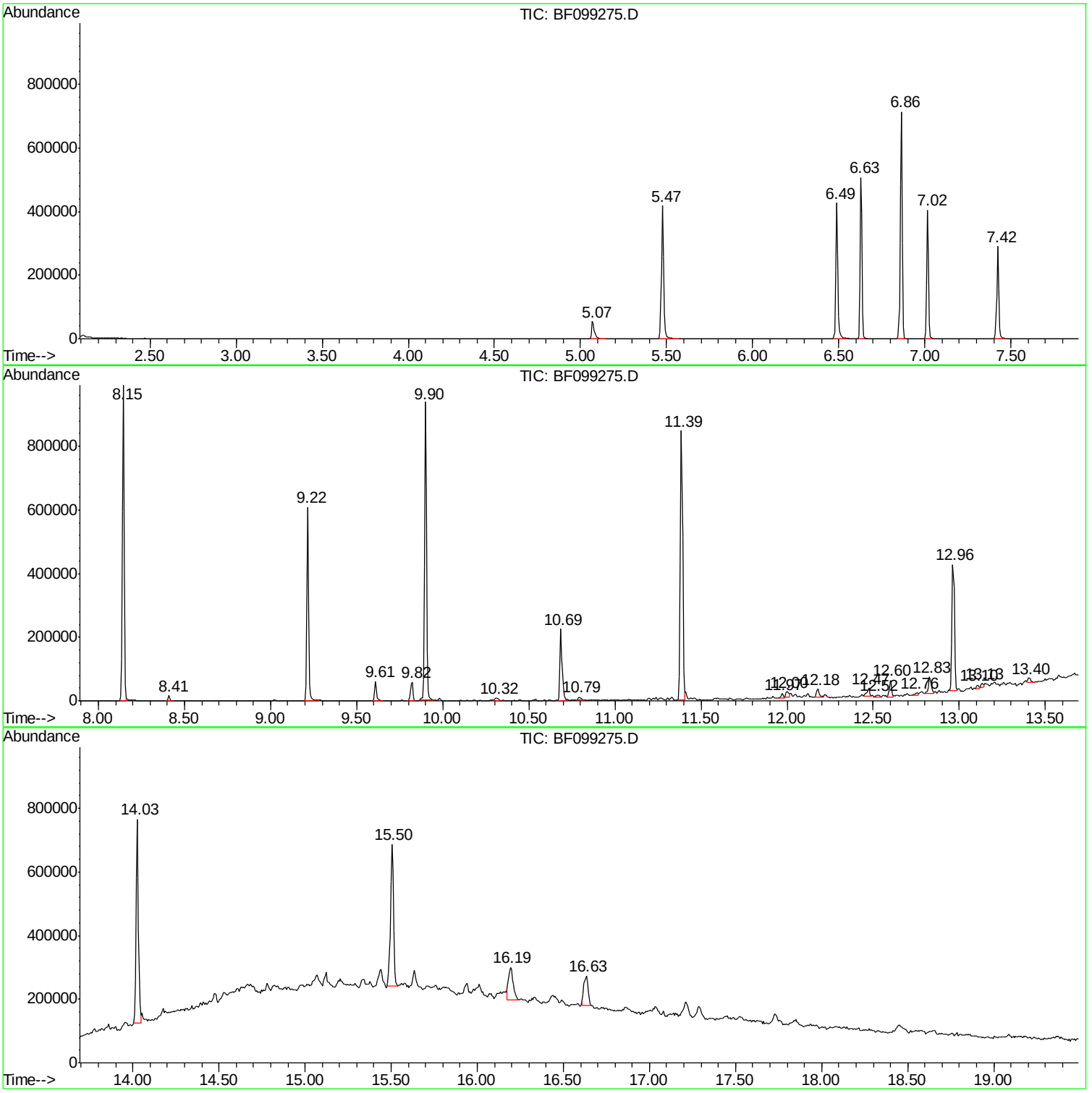
Acq On : 9 Oct 2017 21:13
Operator : SJ/JU
Sample : I5715-13 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-02-100517-E

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100917\
Data File : BF099275.D
Acq On : 9 Oct 2017 21:13
Operator : SJ/JU
Sample : I5715-13 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-02-100517-E

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

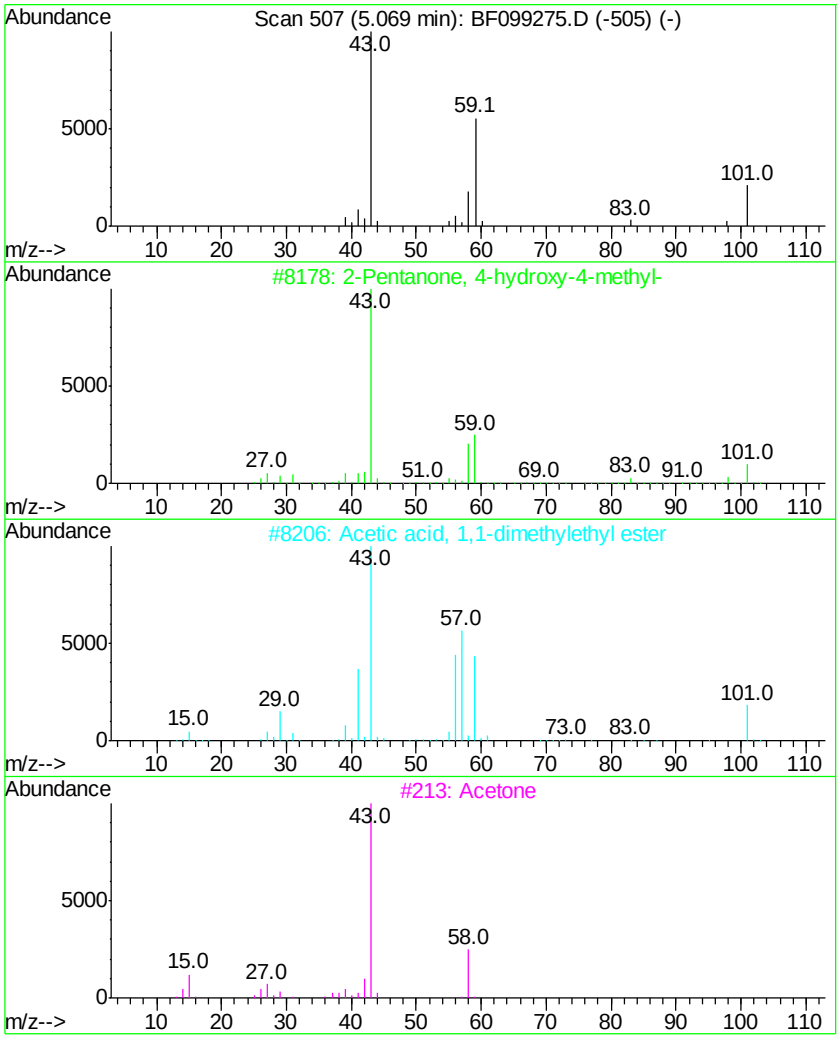
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

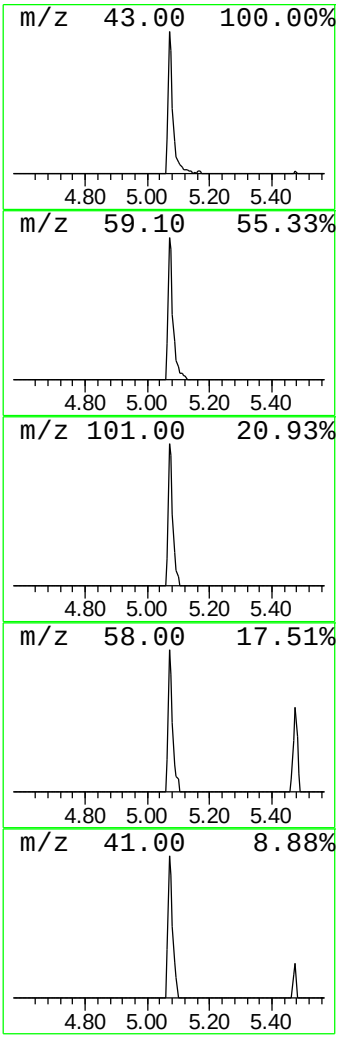
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	2.06 ng	60018	1,4-Dichlorobenzene-d4	6.86

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetone	58	C3H6O	000067-64-1	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9





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

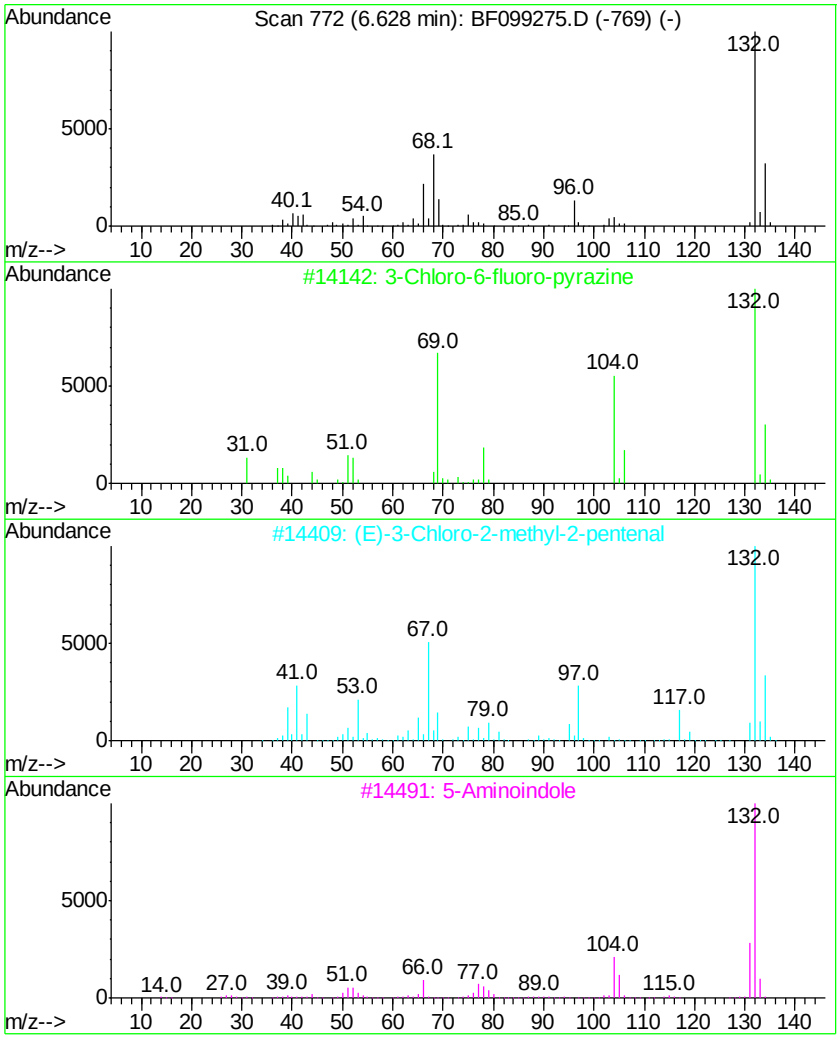
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

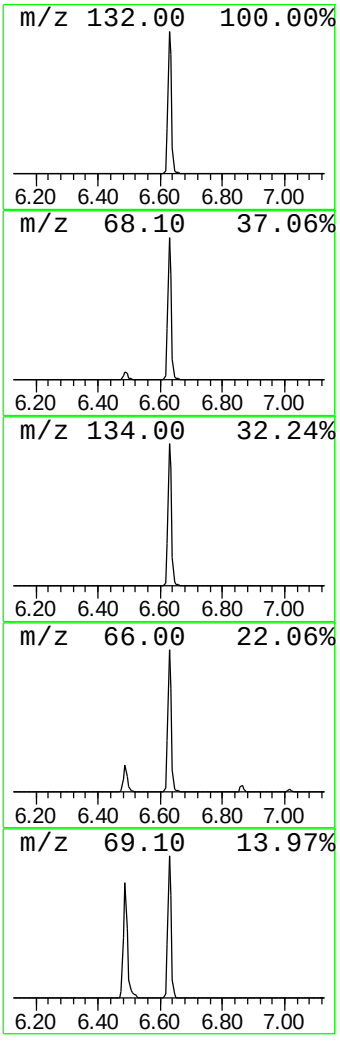
****

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	14.28 ng	415440	1,4-Dichlorobenzene-d4	6.86

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	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Instrument : BNA_F
ClientSampleId : PL-02-100517-E

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

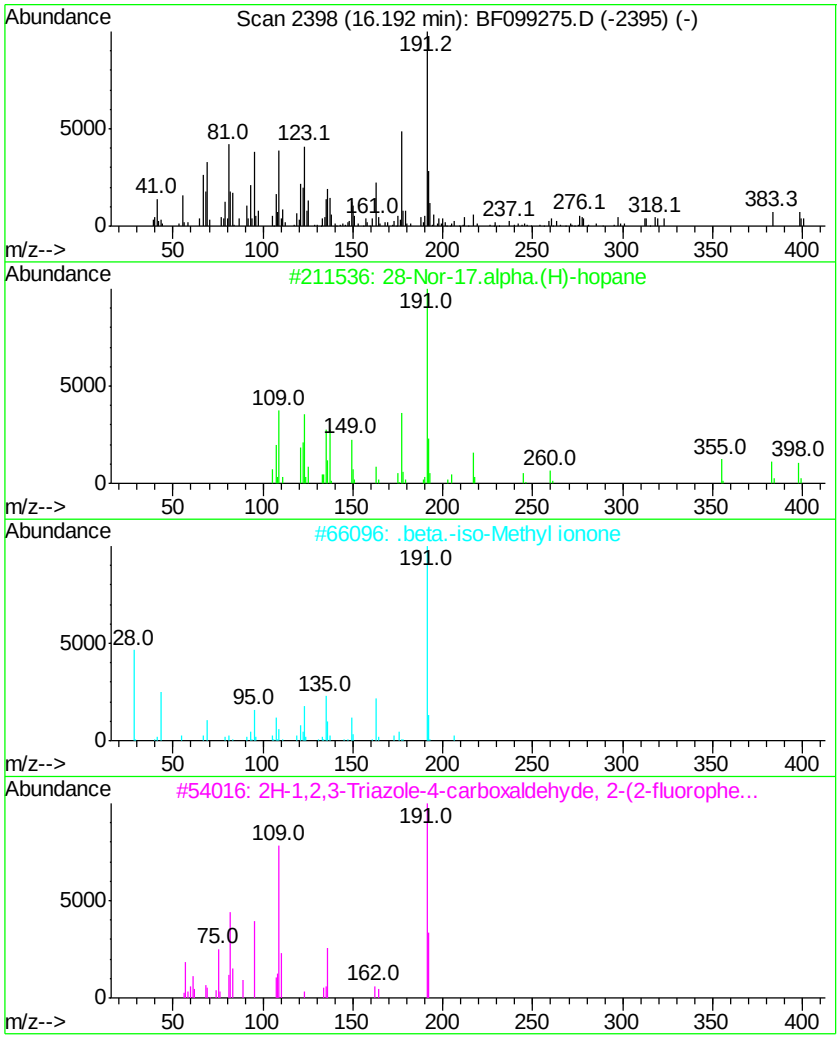
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

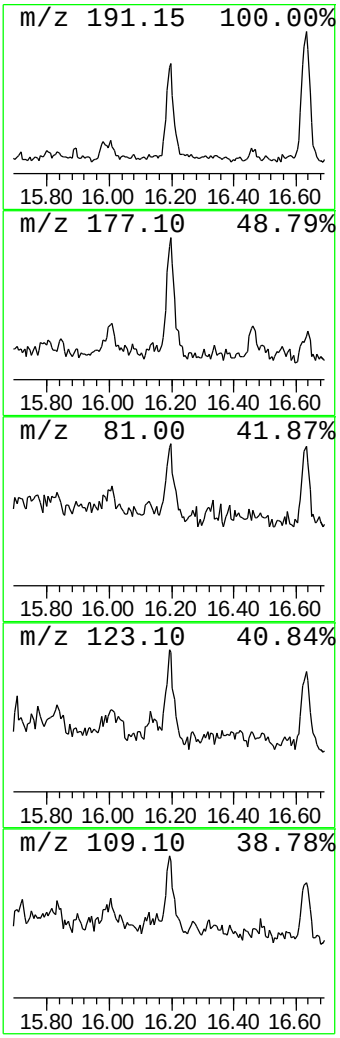
****

Peak Number 5 28-Nor-17.alpha.(H)-hopane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	6.67 ng	184539	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	87
2	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	46
3	2H-1,2,3-Triazole-4-carboxaldehy...	191	C9H6FN3O	051306-43-5	38
4	Spiro[4-oxatricyclo[5.3.0.0(2,6)...	276	C18H28O2	1000156-82-9	35
5	Amiphenazole	191	C9H9N3S	000490-55-1	27





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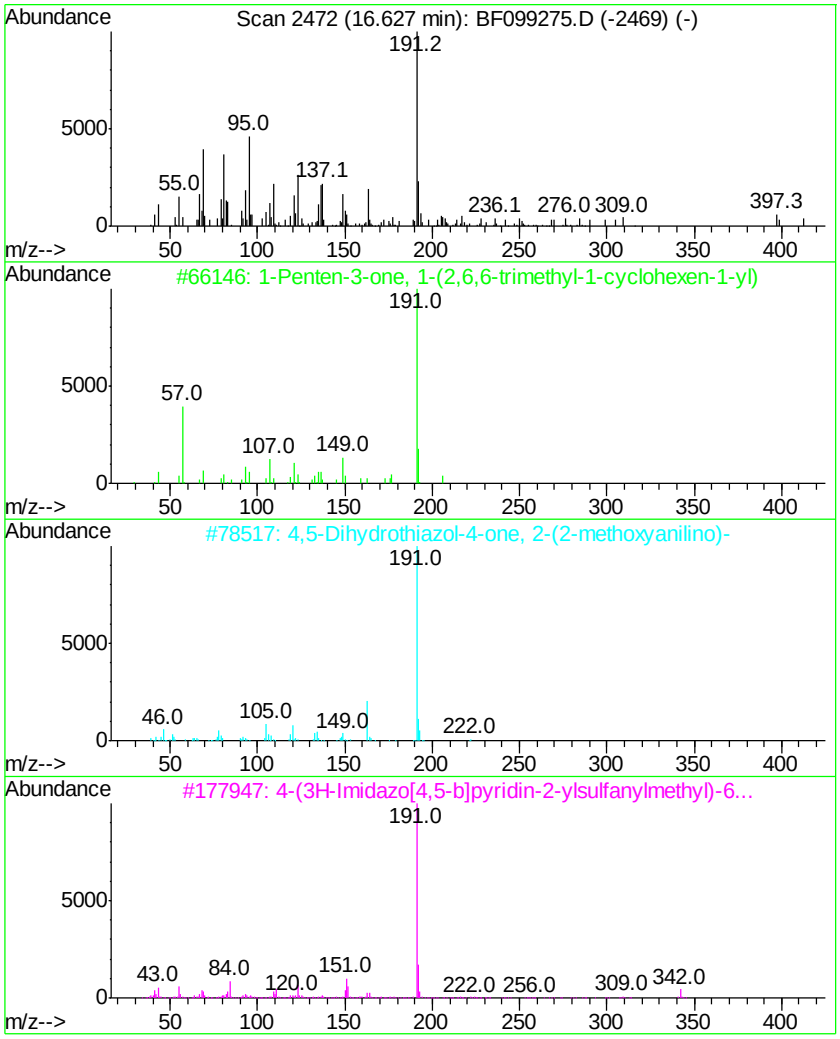
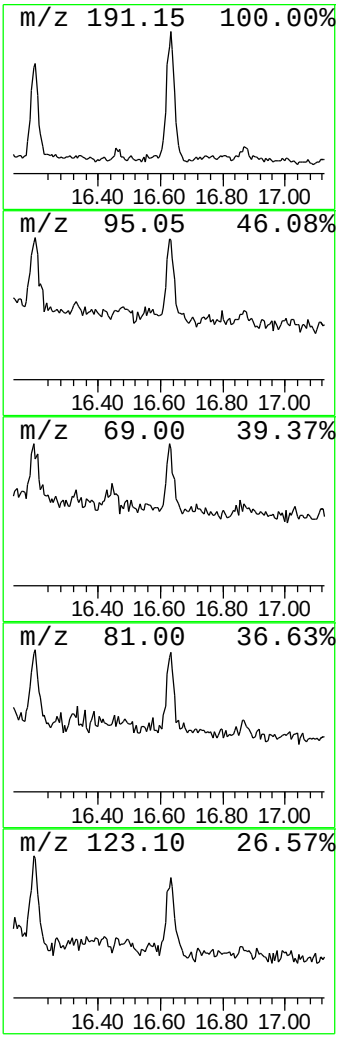
****

Peak Number 6 1-Penten-3-one, 1-(2,6,6-tr... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.63	5.45 ng	150745	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	50
2	4,5-Dihydrothiazol-4-one, 2-(2-m...	222	C10H10N2O2S	022476-61-5	38
3	4-(3H-Imidazo[4,5-b]pyridin-2-yl...	342	C15H18N8S	1000276-08-2	38
4	5-Fluoro-2-trifluoromethylbenzoi...	402	C18H8Cl2F4O2	1000331-61-3	35
5	2-Fluoro-3-trifluoromethylbenzoi...	320	C14H6F6O2	1000357-64-1	27





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.07	2.1	ng	60018	1	6.86	581853	20.0
unknown6.63	6.63	14.3	ng	415440	1	6.86	581853	20.0
28-Nor-17.alpha.(...	16.19	6.7	ng	184539	6	15.50	553647	20.0
1-Penten-3-one, 1...	16.63	5.5	ng	150745	6	15.50	553647	20.0