LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA F\Data\BF-JUN-2018\BF062918\
Data File : BF106985.D
Acq On : 29 Jun 2018 20:40
Operator : JU/SJ
Sample : J3692-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-02

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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	5.184	481	484	490	rBV	63082	72101	3.55%	0.450%
2	5.284	490	501	504	rVB2	18588	47640	2.34%	0.297%
3	5.384	511	518	523	rBV	12982	24143	1.19%	0.151%
4	5.590	550	553	566	rVB	911761	838886	41.28%	5.232%
5	6.531	707	713	717	rBV2	17832	22217	1.09%	0.139%
6	6.590	720	723	735	rVB	597339	580882	28.59%	3.623%
7	6.731	742	747	750	rBV	1628574	1477664	72.72%	9.216%
8	6.948	781	784	788	rBV	482868	419023	20.62%	2.613%
9	7.001	790	793	795	rBV	32086	29026	1.43%	0.181%
10	7.107	807	811	821	rBB	1567304	1477693	72.72%	9.216%
11	7.207	826	828	832	rBV	41537	32187	1.58%	0.201%
12	7.519	876	881	884	rBV	1155993	1140030	56.11%	7.110%
13	7.978	956	959	962	rVB	50320	46902	2.31%	0.293%
14	8.031	962	968	973	rBV7	15212	28019	1.38%	0.175%
15	8.137	983	986	989	rBV	23159	21795	1.07%	0.136%
16	8.237	999	1003	1004	rBV	565457	520743	25.63%	3.248%
17	8.260	1004	1007	1010	rVV	1027151	956592	47.08%	5.966%
18	8.307	1012	1015	1022	rVB	68561	62813	3.09%	0.392%
19	8.595	1061	1064	1070	rVB2	16557	22293	1.10%	0.139%
20	8.948	1120	1124	1127	rBV	129490	107666	5.30%	0.672%
21	9.048	1137	1141	1145	rVB	91760	84041	4.14%	0.524%
22	9.307	1181	1185	1188	rBV	2164755	2031943	100.00%	12.673%
23	9.407	1200	1202	1205	rBV	33160	24419	1.20%	0.152%
24	9.454	1207	1210	1217	rBV	209486	195320	9.61%	1.218%
25	9.648	1239	1243	1245	rBV	26166	26172	1.29%	0.163%
26	9.913	1284	1288	1295	rBV	80499	74400	3.66%	0.464%
27	9.995	1298	1302	1304	rVV	553107	522077	25.69%	3.256%
28	10.025	1304	1307	1310	rVB	235760	176629	8.69%	1.102%
29	10.195	1331	1336	1341	rBV	101641	89083	4.38%	0.556%
30	10.542	1391	1395	1399	rBV	135342	111778	5.50%	0.697%
31	10.631	1408	1410	1413	rVB2	37590	29357	1.44%	0.183%
32	10.748	1426	1430	1433	rBV	51206	50287	2.47%	0.314%
33	10.789	1433	1437	1440	rBV	1234065	1158403	57.01%	7.225%
34	11.078	1482	1486	1491	rBV2	43913	46809	2.30%	0.292%

LSC Area Percent Report

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Acq On : 29 Jun 2018 20:40
Operator : JU/SJ
Sample : J3692-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-02

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.483	1552	1555	1558	rBV	546774	485467	23.89%	3.028%
36	11.507	1558	1559	1563	rVB	190520	123127	6.06%	0.768%
37	11.589	1570	1573	1581	rVB2	34863	40261	1.98%	0.251%
38	11.719	1591	1595	1599	rBV	72482	61553	3.03%	0.384%
39	12.701	1759	1762	1765	rBV	46829	39299	1.93%	0.245%
40	12.936	1796	1802	1808	rBV	29586	31509	1.55%	0.197%
41	13.072	1820	1825	1828	rBV	2029791	1844473	90.77%	11.504%
42	14.136	2002	2006	2010	rBV	568696	496911	24.45%	3.099%
43	15.671	2262	2267	2277	rVB	274227	361991	17.82%	2.258%

Sum of corrected areas: 16033624

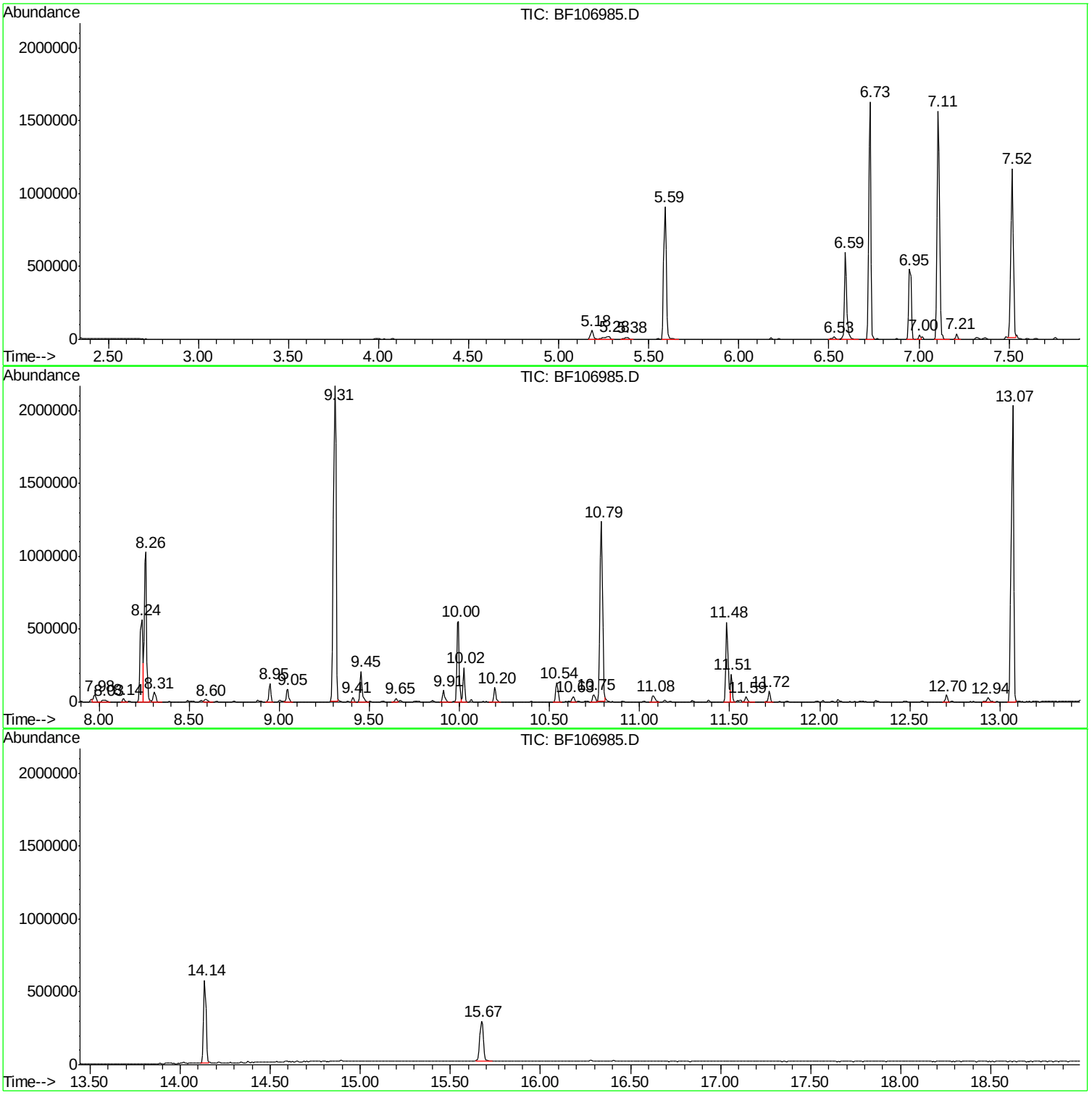
LSC Report - Integrated Chromatogram

Data Path : Z:\svoasrv\HPCHEM1\BNA F\Data\BF-JUN-2018\BF062918\
Data File : BF106985.D
Acq On : 29 Jun 2018 20:40
Operator : JU/SJ
Sample : J3692-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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:\svoasrv\HPCHEM1\BNA F\Data\BF-JUN-2018\BF062918\
Data File : BF106985.D
Acq On : 29 Jun 2018 20:40
Operator : JU/SJ
Sample : J3692-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

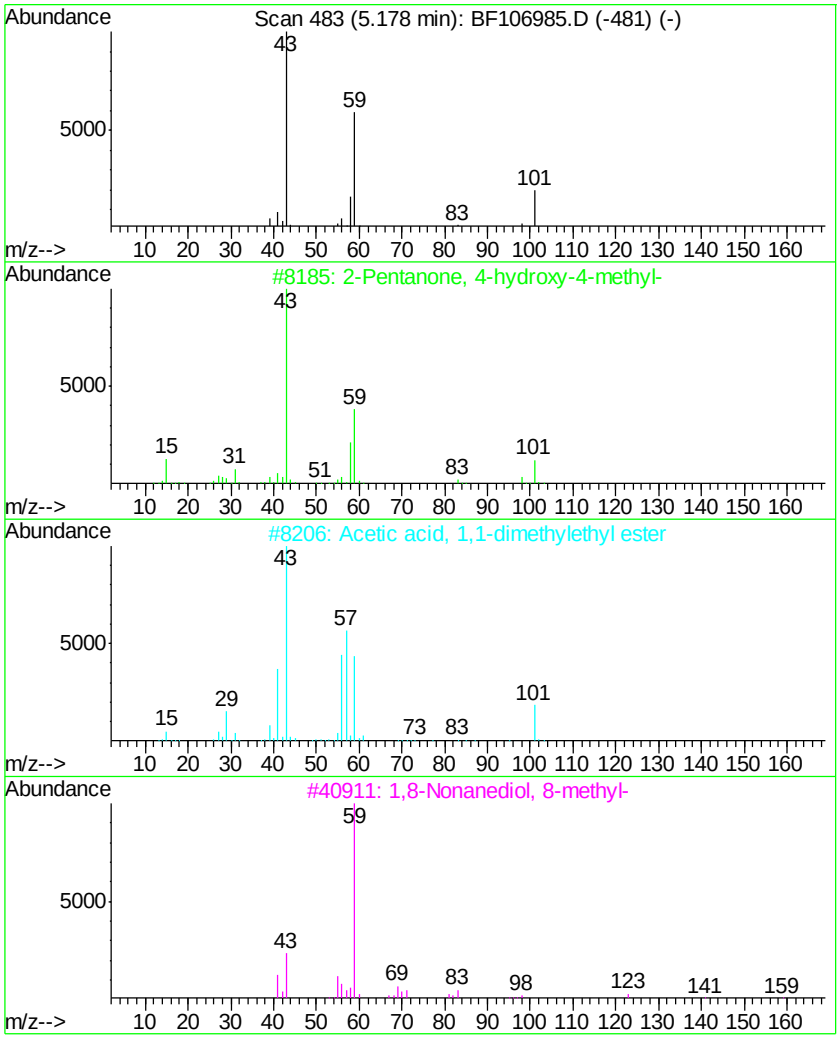
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

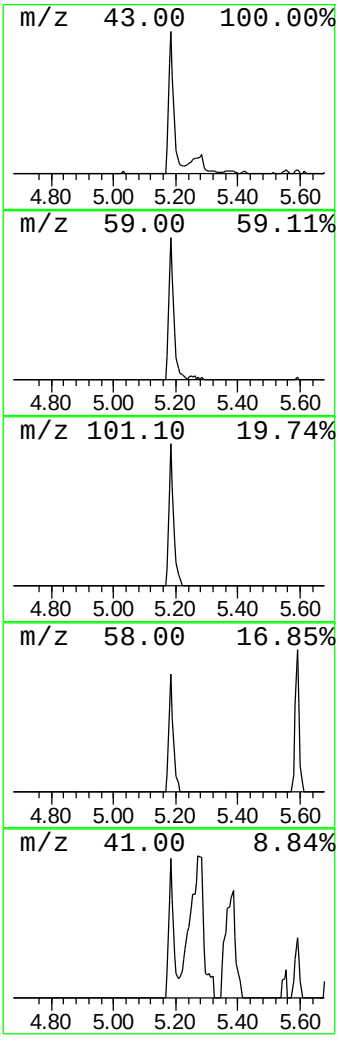
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	3.44 ng	72101	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9





Library Search Compound Report

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Data File : BF106985.D
Acq On : 29 Jun 2018 20:40
Operator : JU/SJ
Sample : J3692-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

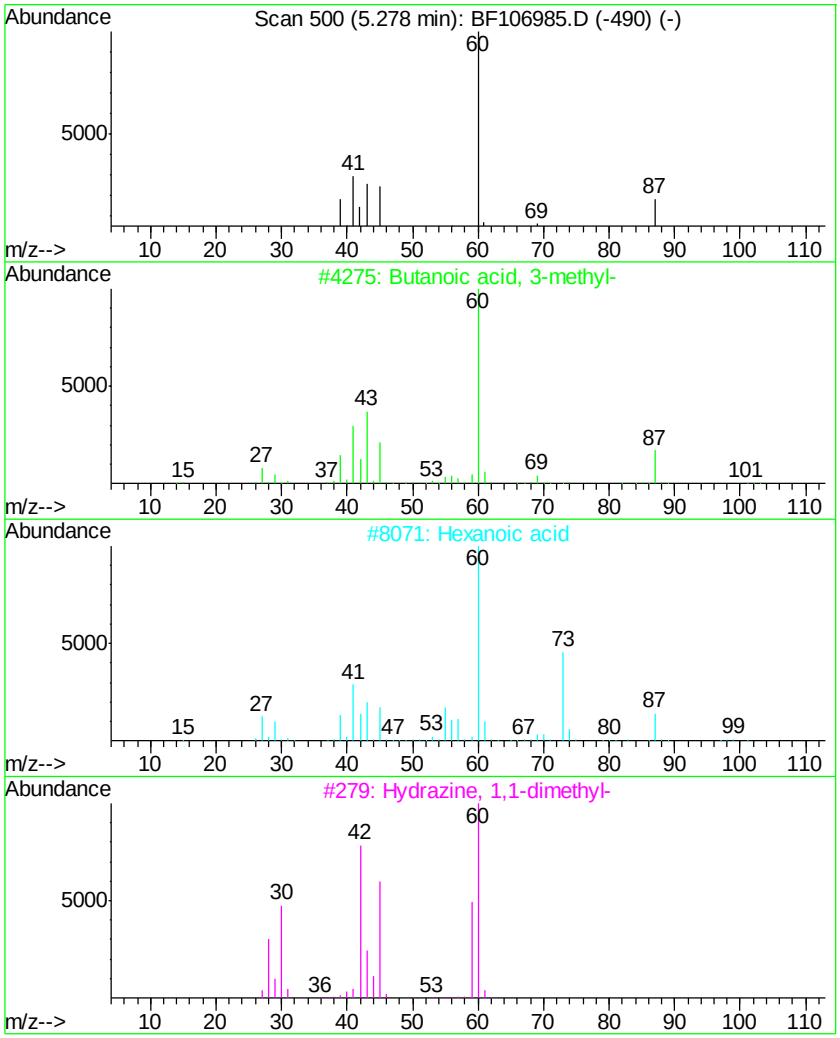
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

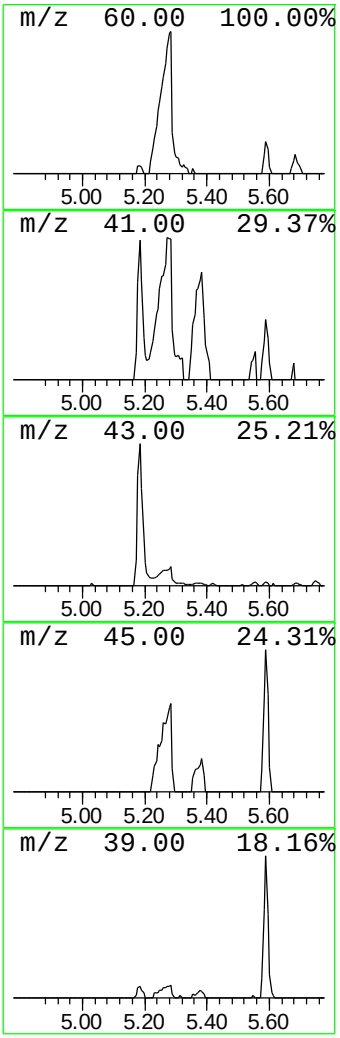
****

Peak Number 2 Butanoic acid, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.28	2.27 ng	47640	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	74
2	Hexanoic acid	116	C6H12O2	000142-62-1	9
3	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	5
4	Urea	60	CH4N2O	000057-13-6	5
5	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	5





Library Search Compound Report

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Data File : BF106985.D
Acq On : 29 Jun 2018 20:40
Operator : JU/SJ
Sample : J3692-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

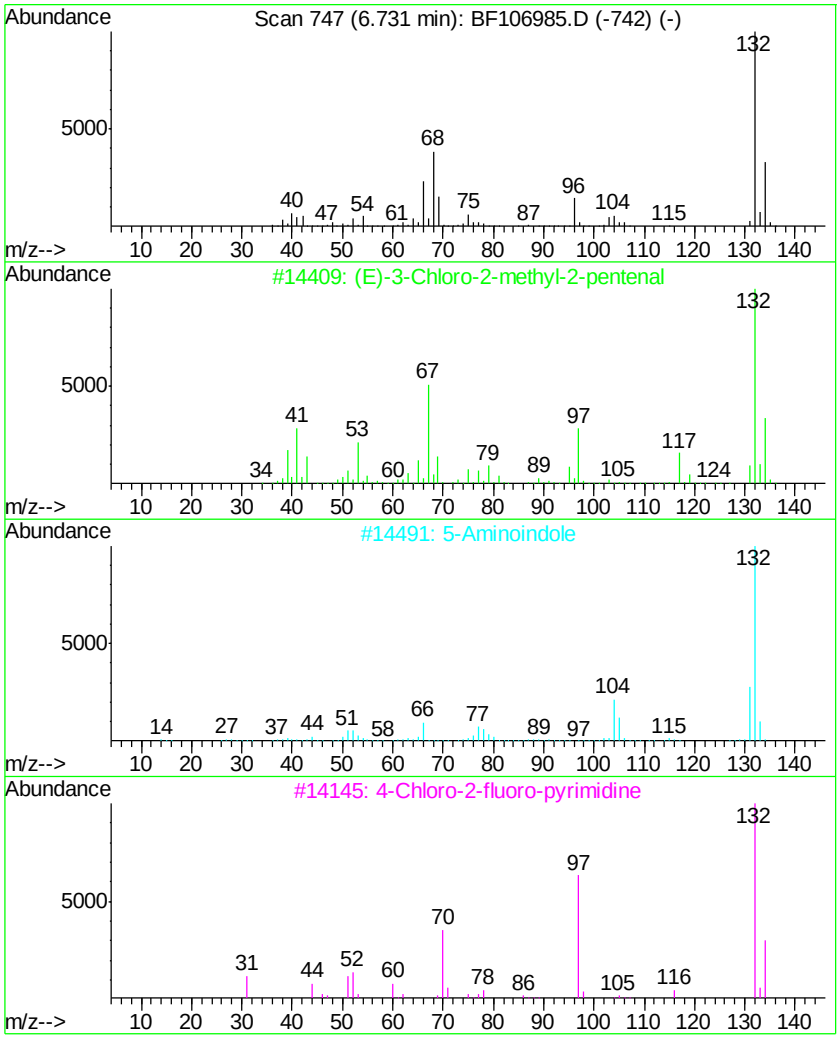
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

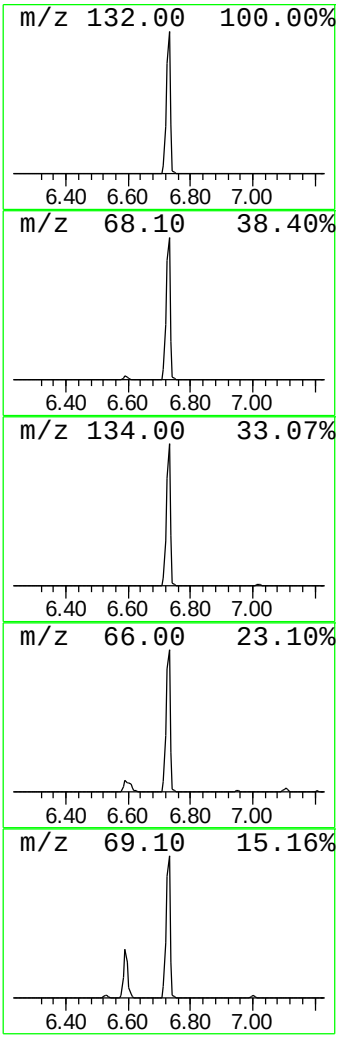
****

Peak Number 3 unknown6.73 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	70.53 ng	1477660	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

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Data File : BF106985.D
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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-02

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

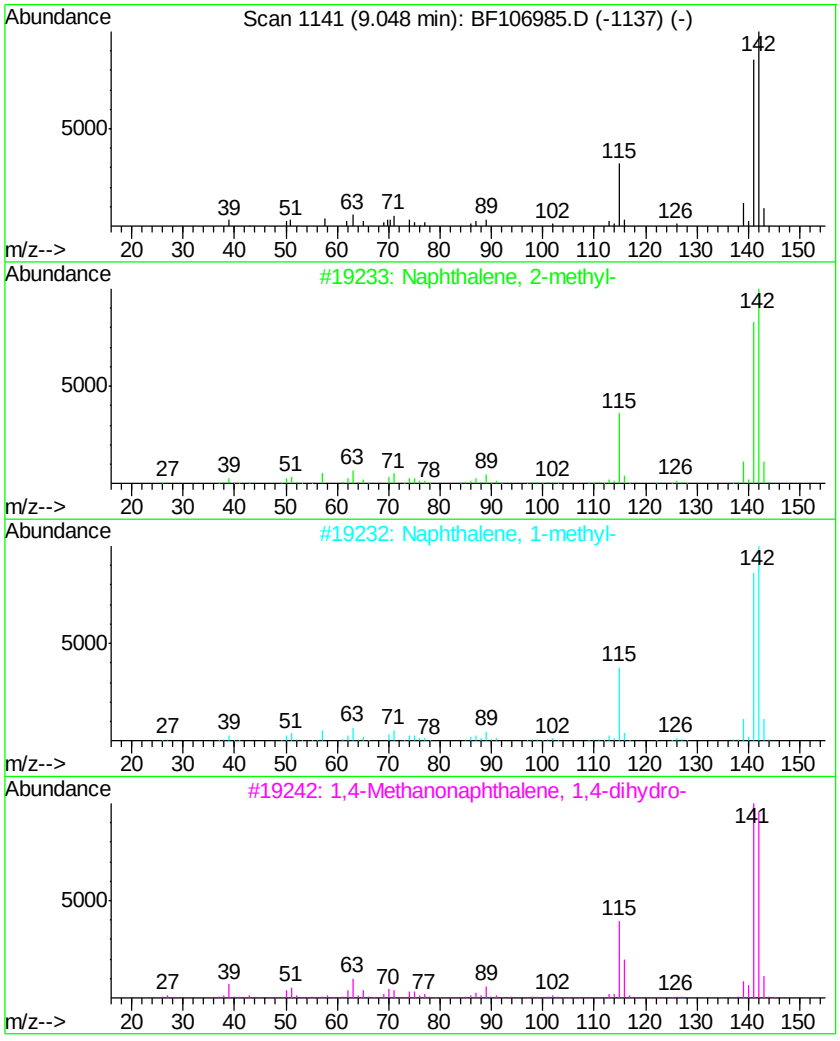
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

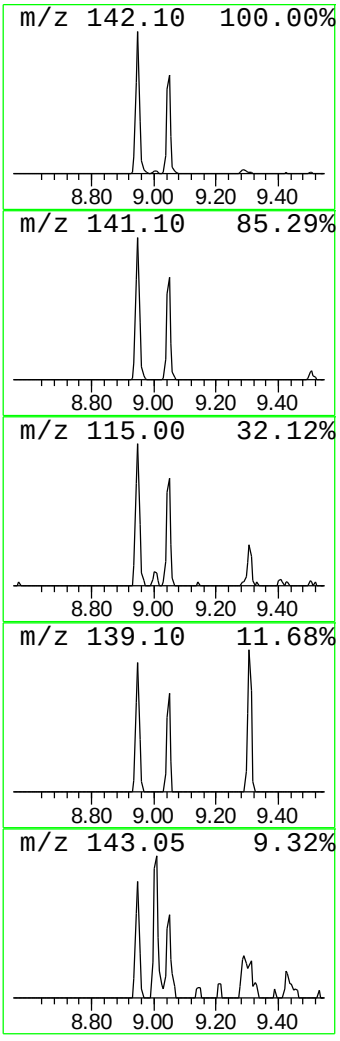
****

Peak Number 5 Naphthalene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.05	3.23 ng	84041	Naphthalene-d8	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	97
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	59





Library Search Compound Report

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Sample : J3692-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

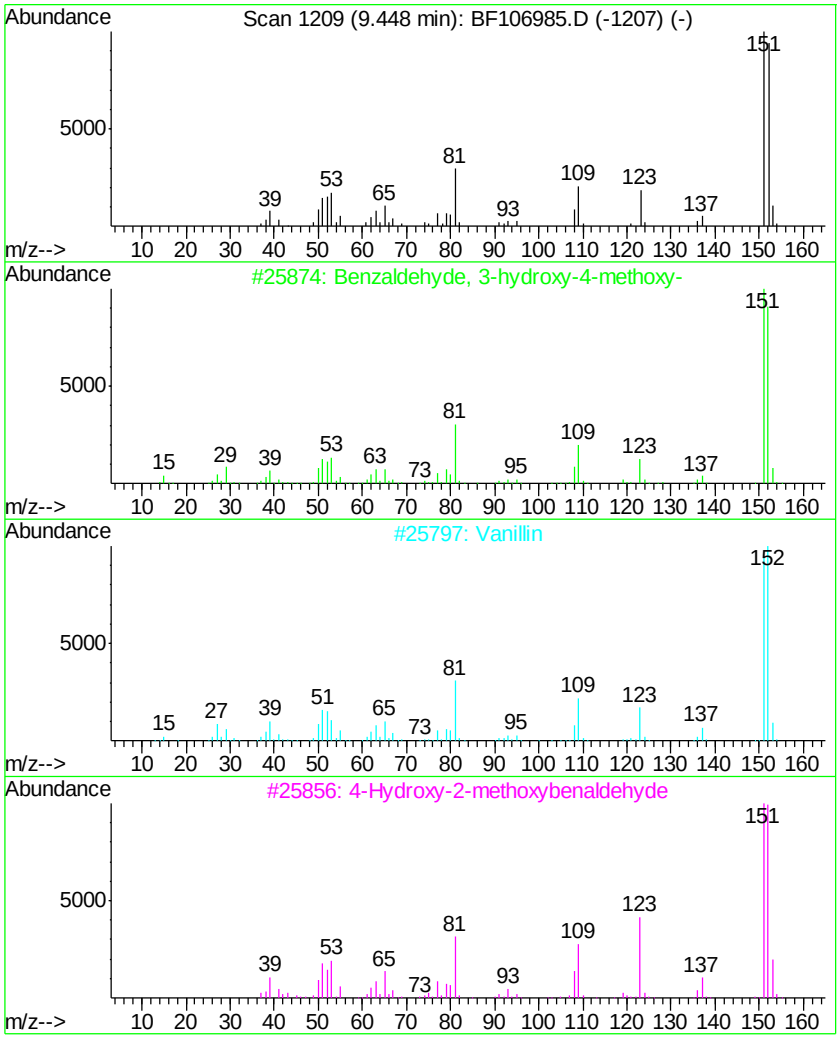
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

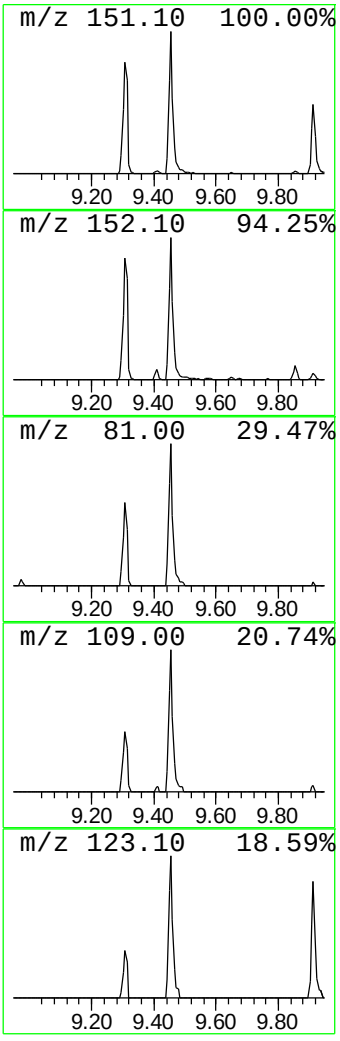
****

Peak Number 6 Benzaldehyde, 3-hydroxy-4-m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.45	7.48 ng	195320	Acenaphthene-d10	9.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	97
2	Vanillin	152	C8H8O3	000121-33-5	97
3	4-Hydroxy-2-methoxybenaldehyde	152	C8H8O3	018278-34-7	81
4	Benzaldehyde, 2-hydroxy-4-methoxy-	152	C8H8O3	000673-22-3	80
5	Benzaldehyde, 3-(chloroacetoxy)-...	228	C10H9ClO4	066267-38-7	78





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ClientSampleId : WC-02

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

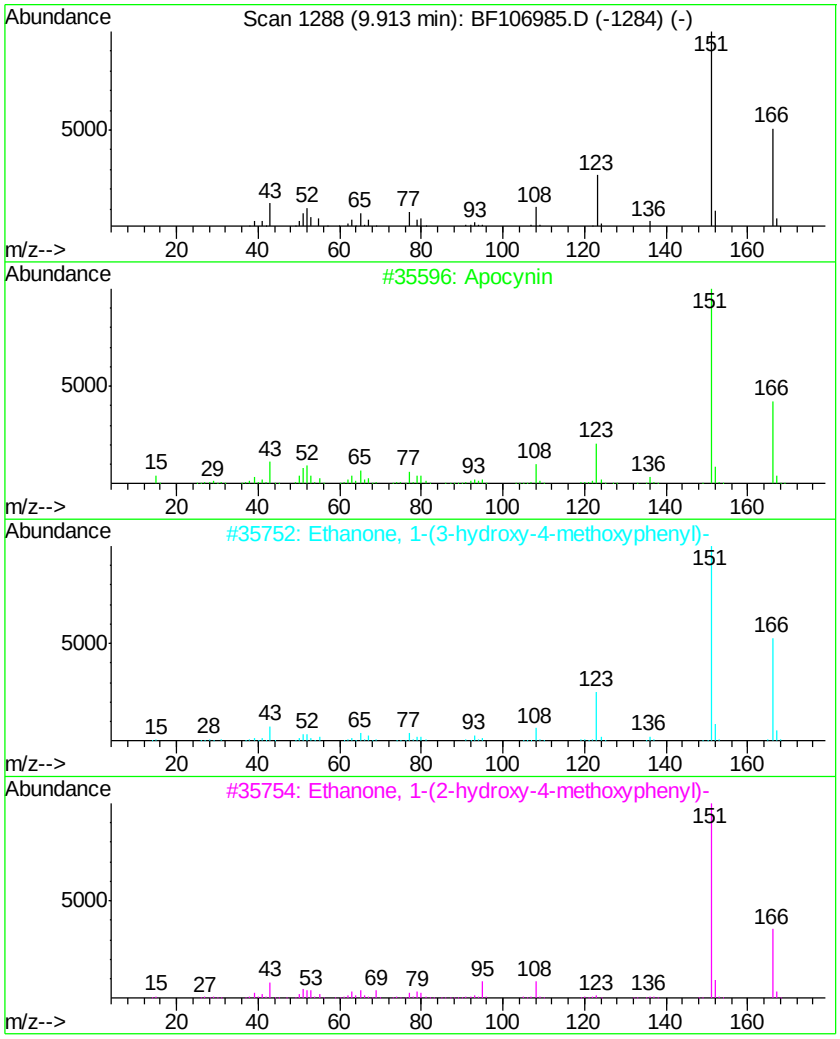
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

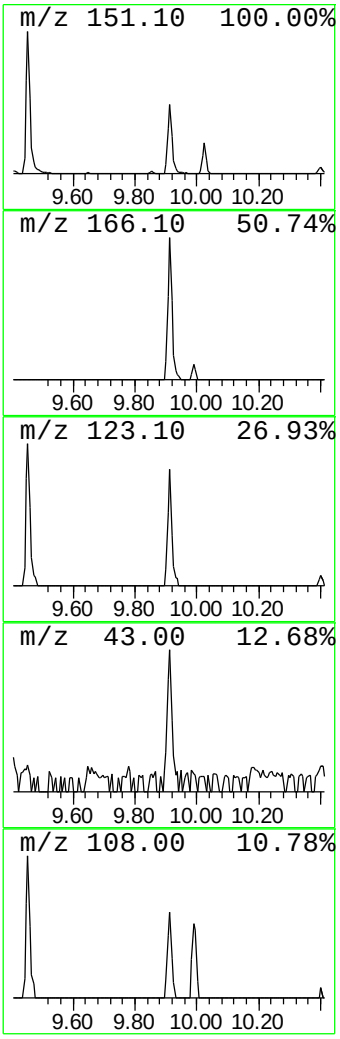
****

Peak Number 7 Apocynin Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.91	2.85 ng	74400	Acenaphthene-d10	9.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Apocynin	166	C9H10O3	000498-02-2	95
2	Ethanone, 1-(3-hydroxy-4-methoxy...	166	C9H10O3	006100-74-9	91
3	Ethanone, 1-(2-hydroxy-4-methoxy...	166	C9H10O3	000552-41-0	81
4	Ethanone, 1-(2-hydroxy-5-methoxy...	166	C9H10O3	000705-15-7	80
5	4-Acetoxy-3-methoxyacetophenone	208	C11H12O4	054771-60-7	64





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
2-Pentanone, 4-hy...	5.18	3.4	ng	72101	1	6.95	419023	20.0
Butanoic acid, 3-...	5.28	2.3	ng	47640	1	6.95	419023	20.0
unknown6.73	6.73	70.5	ng	1477660	1	6.95	419023	20.0
Naphthalene, 1-me...	9.05	3.2	ng	84041	2	8.24	520743	20.0
Benzaldehyde, 3-h...	9.45	7.5	ng	195320	3	9.99	522077	20.0
Apocynin	9.91	2.9	ng	74400	3	9.99	522077	20.0