LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012818\
Data File : BF102576.D
Acq On : 28 Jan 2018 23:45
Operator : SJ/JU
Sample : J1290-14 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-45-0-2.0

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-BF012218.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	4.898	475	478	485	rBV	37465	48608	2.43%	0.215%
2	5.322	546	550	568	rBV	1747665	1865854	93.41%	8.248%
3	6.357	722	726	744	rBV	1801395	1997488	100.00%	8.830%
4	6.487	744	748	761	rVB	2137148	1957193	97.98%	8.652%
5	6.716	783	787	795	rBV	959203	906106	45.36%	4.005%
6	6.869	809	813	821	rBV	1768189	1516607	75.93%	6.704%
7	7.281	879	883	894	rBV	1235645	1114932	55.82%	4.929%
8	7.457	910	913	918	rVB	23071	22285	1.12%	0.099%
9	7.998	1001	1005	1021	rVB	1363388	1239402	62.05%	5.479%
10	9.069	1184	1187	1196	rBV	2186171	1931976	96.72%	8.540%
11	9.145	1198	1200	1203	rVB	32929	29831	1.49%	0.132%
12	9.398	1240	1243	1248	rBV4	55816	55234	2.77%	0.244%
13	9.469	1248	1255	1261	rVV	264775	258662	12.95%	1.143%
14	9.522	1261	1264	1274	rVV	150948	239307	11.98%	1.058%
15	9.610	1277	1279	1283	rVV	64485	58431	2.93%	0.258%
16	9.675	1287	1290	1294	rVV	88514	68838	3.45%	0.304%
17	9.716	1294	1297	1299	rVV3	21505	25081	1.26%	0.111%
18	9.751	1299	1303	1307	rVV	1346393	1195509	59.85%	5.285%
19	9.780	1307	1308	1312	rVB	38850	28903	1.45%	0.128%
20	9.998	1341	1345	1348	rVB3	22951	22895	1.15%	0.101%
21	10.175	1372	1375	1378	rVB	105885	78074	3.91%	0.345%
22	10.298	1393	1396	1401	rVB2	21444	26701	1.34%	0.118%
23	10.392	1408	1412	1417	rBV3	24018	34925	1.75%	0.154%
24	10.539	1434	1437	1447	rBV	818083	850504	42.58%	3.760%
25	10.645	1452	1455	1465	rVB	84407	99530	4.98%	0.440%
26	10.839	1485	1488	1492	rBV6	15028	23814	1.19%	0.105%
27	11.092	1528	1531	1534	rBV2	41553	38988	1.95%	0.172%
28	11.239	1552	1556	1558	rBV	949673	931957	46.66%	4.120%
29	11.257	1558	1559	1566	rVV	297965	267570	13.40%	1.183%
30	11.316	1566	1569	1571	rVB	73800	64732	3.24%	0.286%
31	11.474	1592	1596	1601	rBV2	28956	41309	2.07%	0.183%
32	11.739	1638	1641	1643	rBV	54701	48643	2.44%	0.215%
33	11.769	1643	1646	1649	rVV	65560	60481	3.03%	0.267%
34	11.816	1652	1654	1656	rVV	31980	24793	1.24%	0.110%

LSC Area Percent Report

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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-BF012218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.851	1656	1660	1662	rVV2	81745	90416	4.53%	0.400%
36	11.869	1662	1663	1669	rVB	43938	41038	2.05%	0.181%
37	11.927	1669	1673	1675	rBV4	24324	27259	1.36%	0.120%
38	12.033	1684	1691	1693	rBV2	45280	58613	2.93%	0.259%
39	12.069	1695	1697	1702	rVB5	26606	28424	1.42%	0.126%
40	12.286	1731	1734	1737	rBV	56589	62075	3.11%	0.274%
41	12.327	1737	1741	1743	rVV4	39926	60289	3.02%	0.267%
42	12.380	1746	1750	1753	rBV3	41957	55459	2.78%	0.245%
43	12.451	1756	1762	1766	rVB	540006	481102	24.09%	2.127%
44	12.680	1795	1801	1806	rBV	481857	552053	27.64%	2.440%
45	12.821	1821	1825	1828	rBV	1312752	1189787	59.56%	5.259%
46	12.992	1850	1854	1855	rBV4	43483	60448	3.03%	0.267%
47	13.010	1855	1857	1859	rVB	65226	52854	2.65%	0.234%
48	13.074	1866	1868	1870	rBV	33176	27788	1.39%	0.123%
49	13.110	1872	1874	1877	rVV2	41963	43849	2.20%	0.194%
50	13.204	1888	1890	1893	rBV	40055	36661	1.84%	0.162%
51	13.233	1893	1895	1897	rBV	47983	44072	2.21%	0.195%
52	13.627	1960	1962	1964	rBV	58231	46415	2.32%	0.205%
53	13.716	1974	1977	1982	rVB2	148596	207469	10.39%	0.917%
54	13.880	2000	2005	2008	rBV2	924676	1034693	51.80%	4.574%
55	13.904	2008	2009	2017	rVB	255650	178374	8.93%	0.788%
56	14.904	2176	2179	2182	rBV	186943	236489	11.84%	1.045%
57	15.310	2245	2248	2253	rBV	445892	541231	27.10%	2.392%
58	15.721	2315	2318	2323	rVB	203583	289989	14.52%	1.282%

Sum of corrected areas: 22622010

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012818\
Data File : BF102576.D
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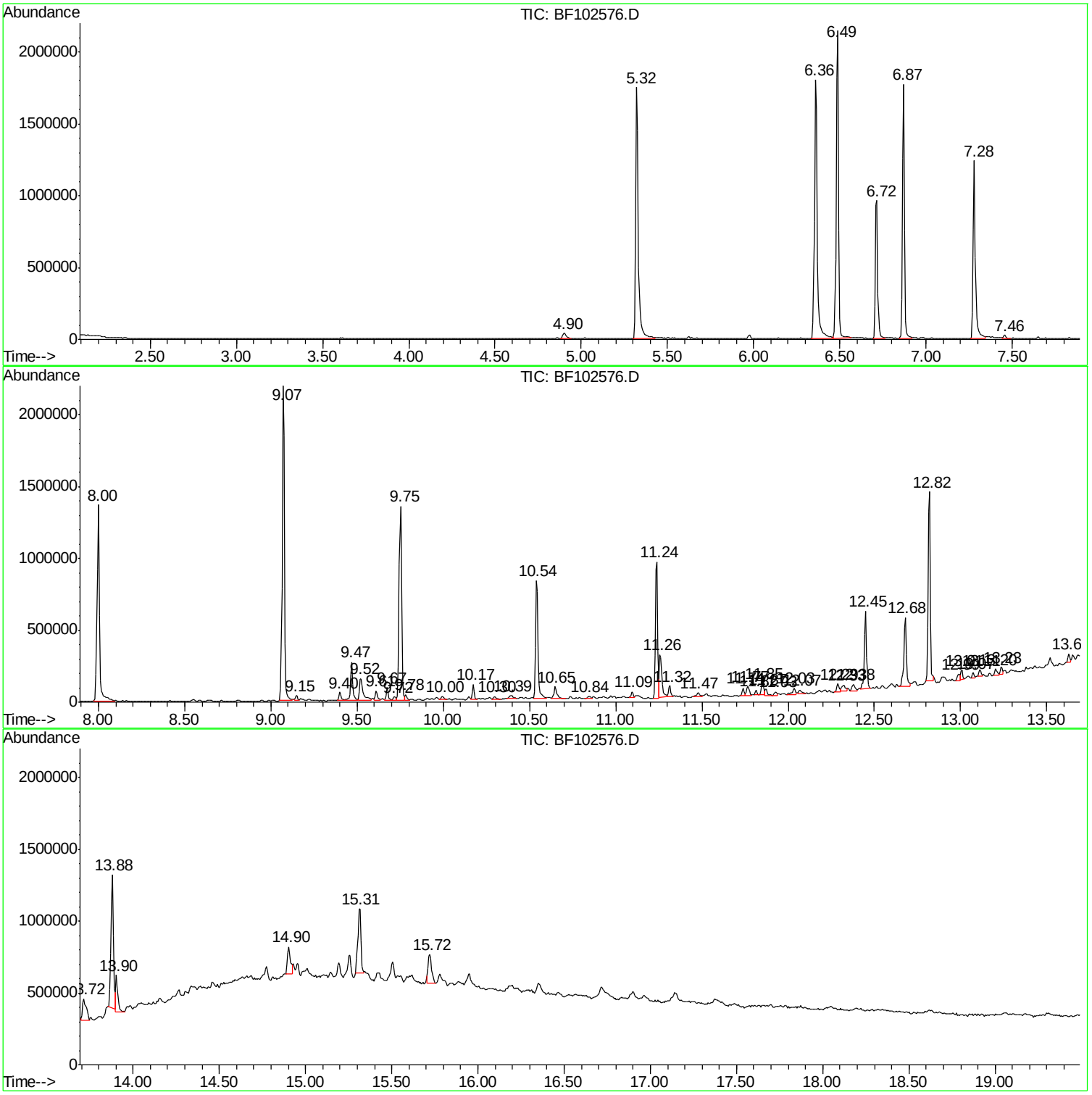
Operator : SJ/JU
Sample : J1290-14 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-45-0-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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\BF012818\
Data File : BF102576.D
Acq On : 28 Jan 2018 23:45
Operator : SJ/JU
Sample : J1290-14 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-45-0-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

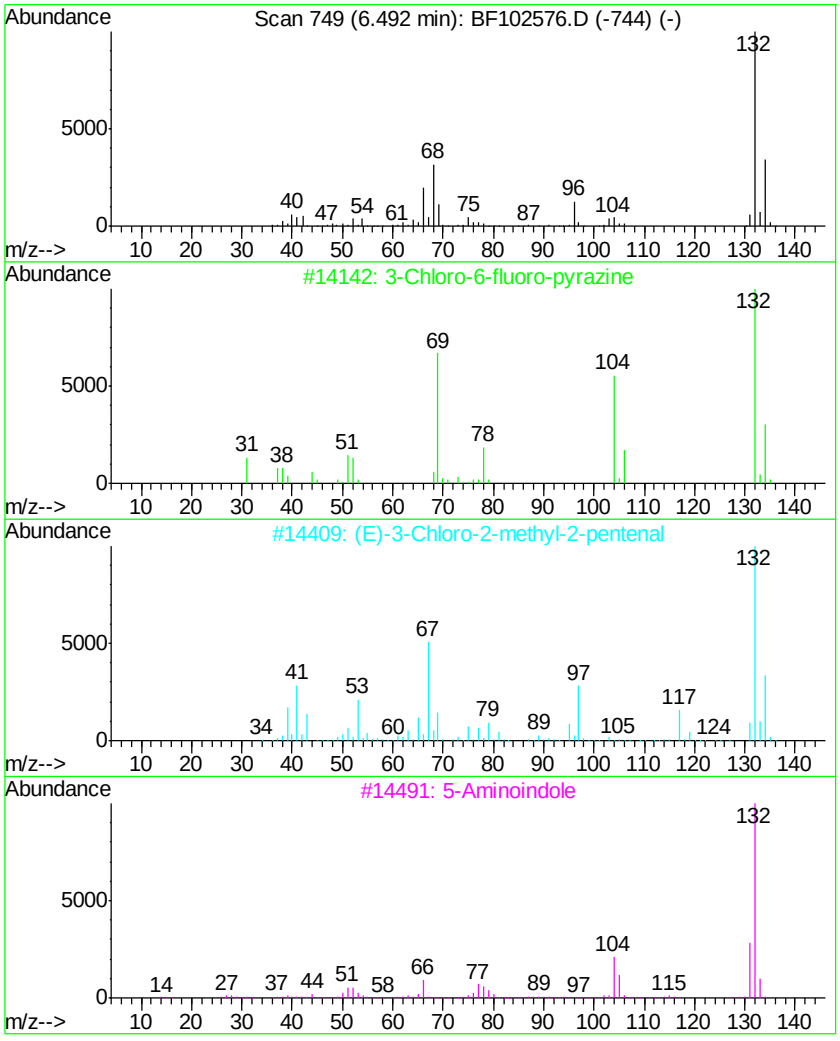
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

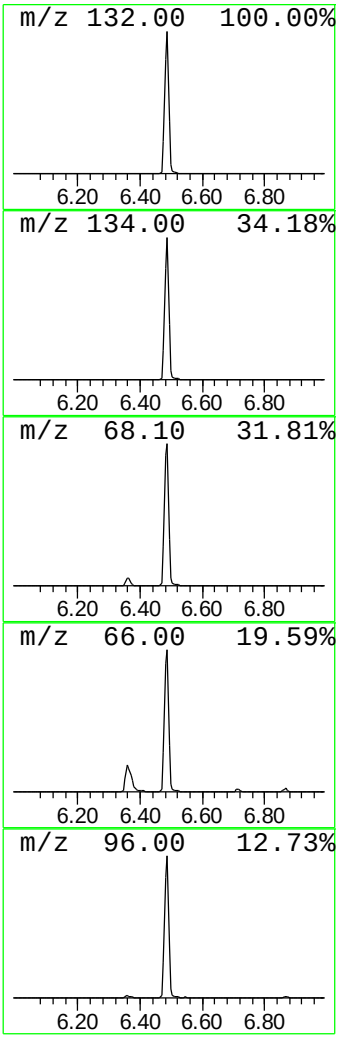
****

Peak Number 1 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	43.20 ng	1957190	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Xenon	132	Xe	007440-63-3	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Sample : J1290-14 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-45-0-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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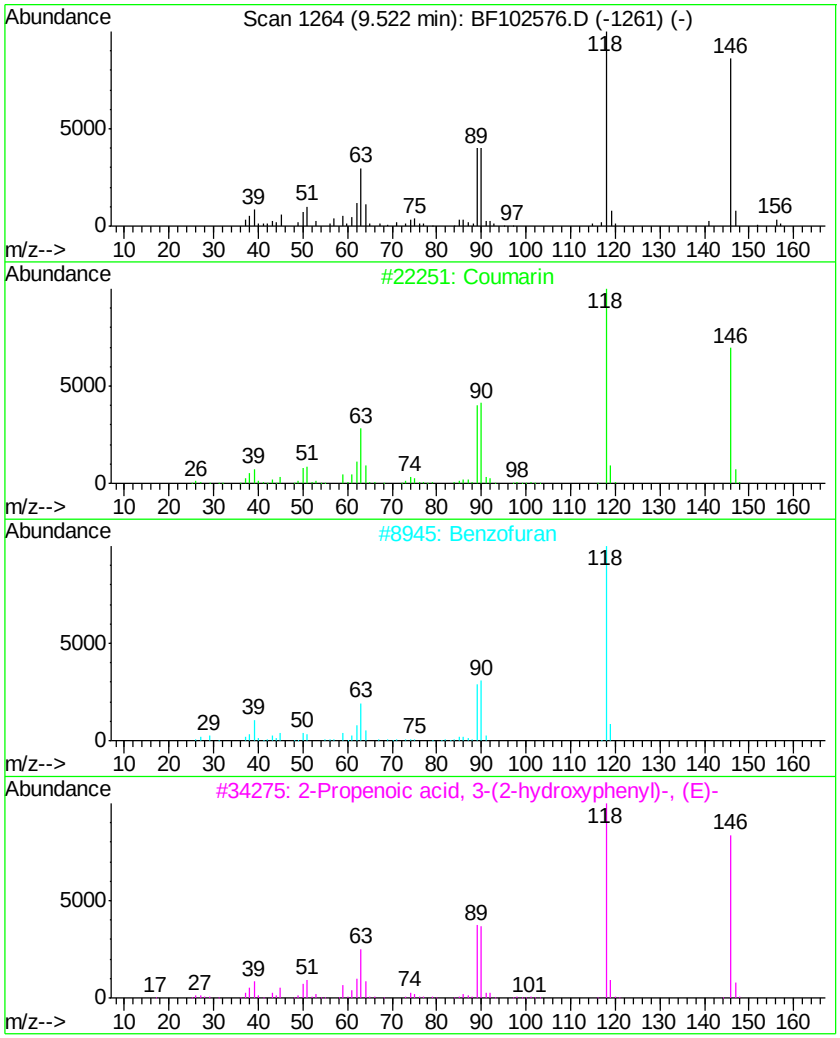
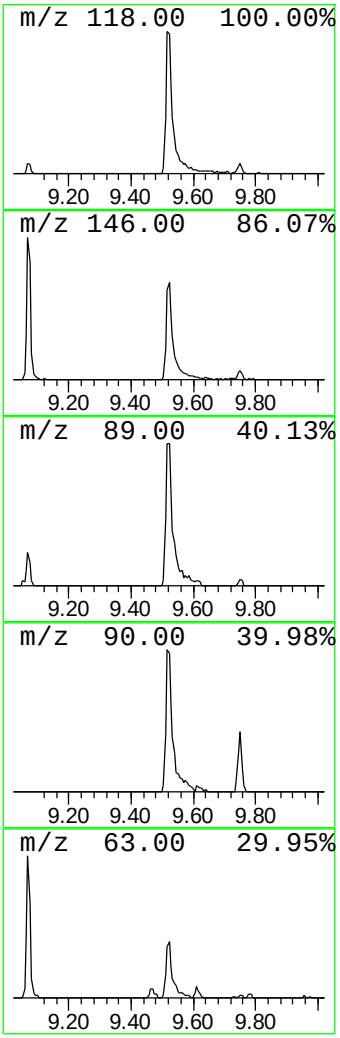
Peak Number 3 Coumarin Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.52	4.00 ng	239307	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Coumarin	146	C9H6O2	000091-64-5	98
2	Benzofuran	118	C8H6O	000271-89-6	93
3	2-Propenoic acid, 3-(2-hydroxyph...	164	C9H8O3	000614-60-8	91
4	1H-Tetrazole, 5-phenyl-	146	C7H6N4	018039-42-4	58
5	1(2H)-Naphthalenone, 3,4-dihydro-	146	C10H10O	000529-34-0	50





Library Search Compound Report

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Acq On : 28 Jan 2018 23:45
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Sample : J1290-14 2X
Misc :
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Instrument : BNA_F
ClientSampleId : SB-45-0-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
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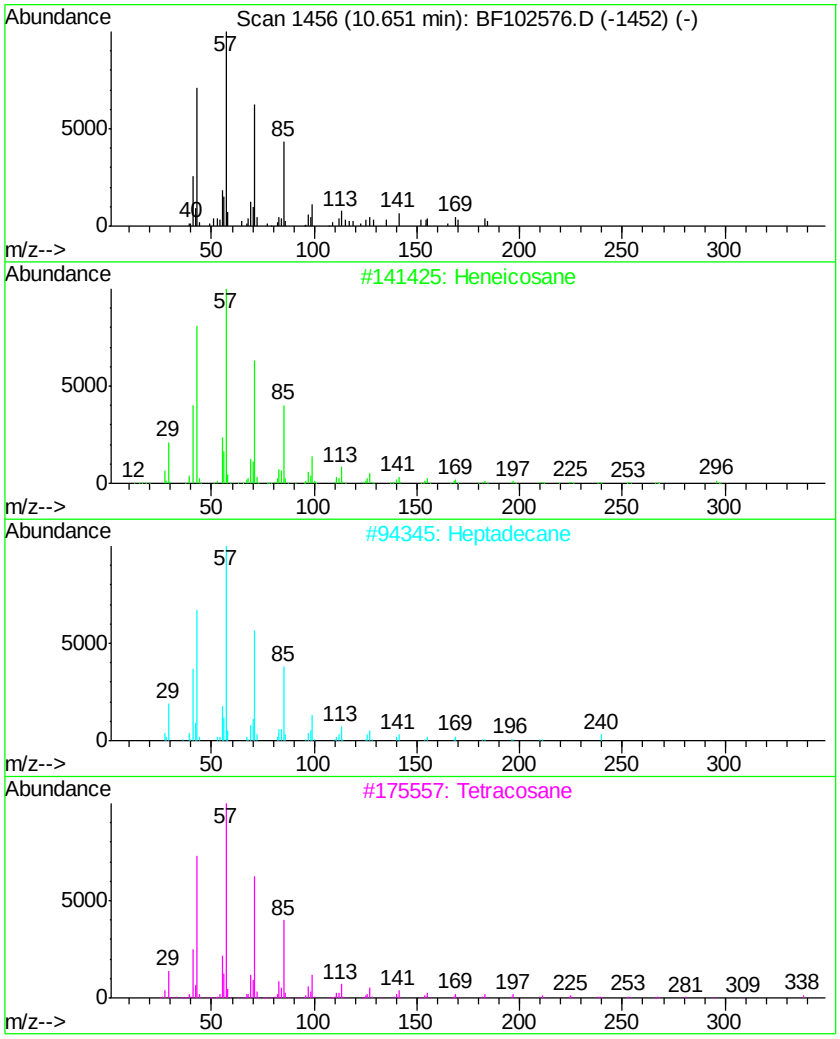
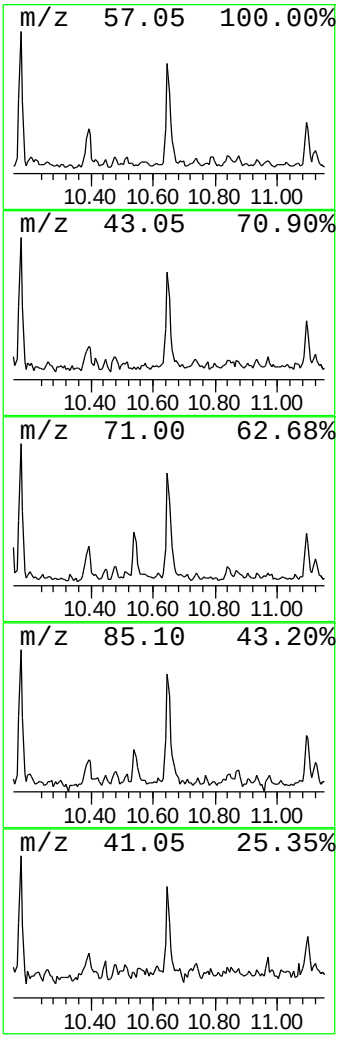
Peak Number 4 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	2.14 ng	99530	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Eicosane	282	C20H42	000112-95-8	90
5	Octadecane	254	C18H38	000593-45-3	90





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Sample : J1290-14 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-45-0-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

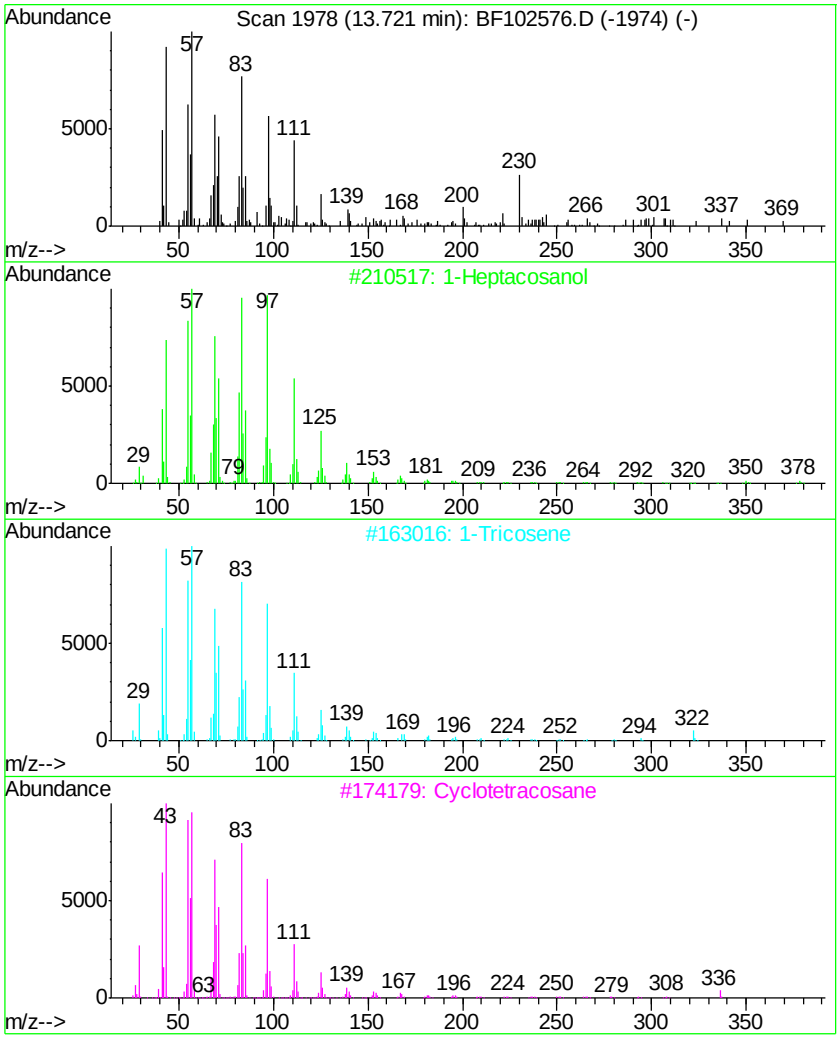
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

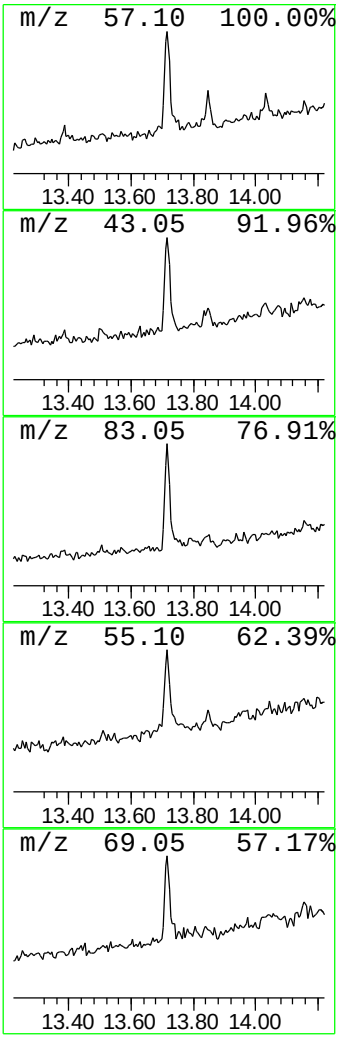
****

Peak Number 5 1-Heptacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	4.01 ng	207469	Chrysene-d12	13.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	91
2	1-Tricosene	322	C23H46	018835-32-0	91
3	Cyclotetracosane	336	C24H48	000297-03-0	87
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	83
5	E-14-Hexadecenal	238	C16H30O	330207-53-9	78





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Misc :
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Instrument : BNA_F
ClientSampleId : SB-45-0-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

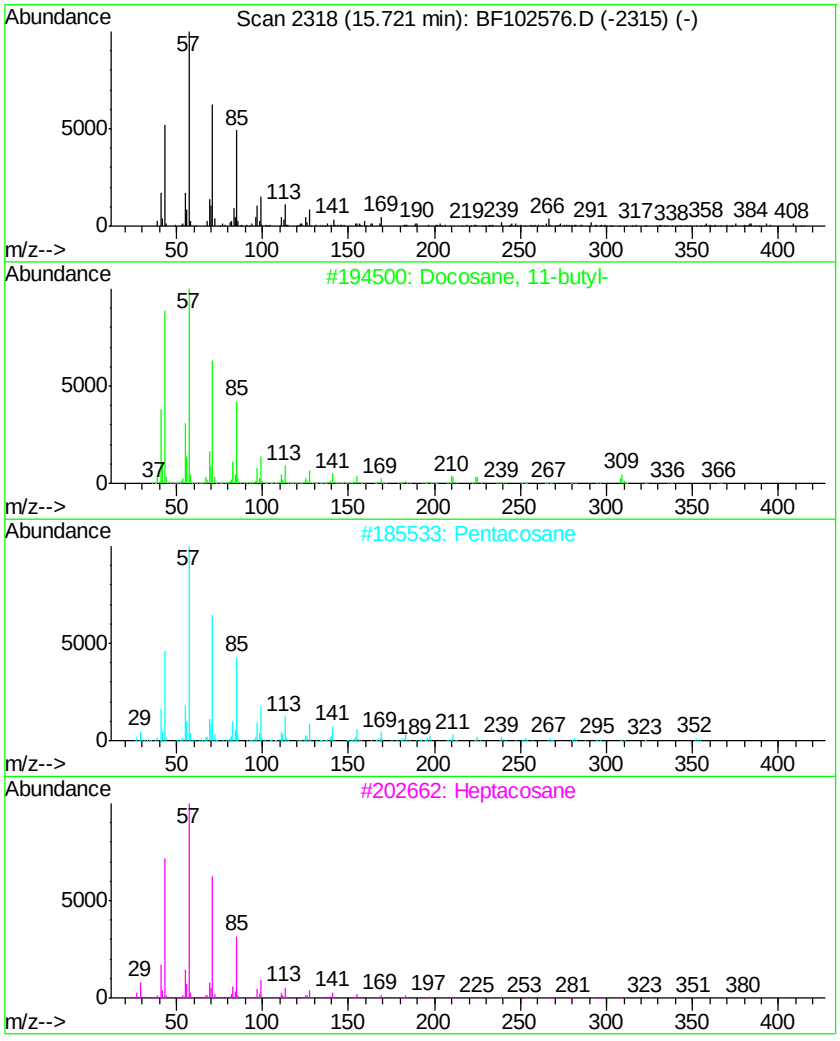
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

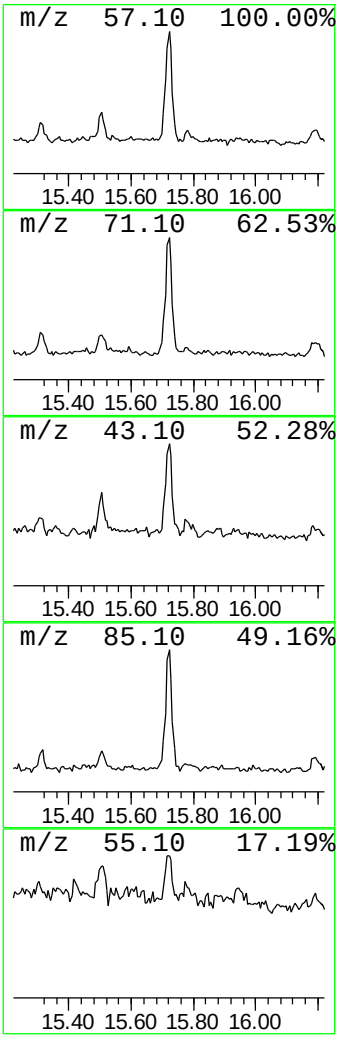
****

Peak Number 6 Docosane, 11-butyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	10.72 ng	289989	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 11-butyl-	366	C26H54	013475-76-8	90
2	Pentacosane	352	C25H52	000629-99-2	87
3	Heptacosane	380	C27H56	000593-49-7	86
4	Triacontane	422	C30H62	000638-68-6	86
5	Docosane	310	C22H46	000629-97-0	86





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
unknown6.49	6.49	43.2	ng	1957190	1	6.72	906106	20.0
Coumarin	9.52	4.0	ng	239307	3	9.75	1195510	20.0
Heneicosane	10.65	2.1	ng	99530	4	11.24	931957	20.0
1-Heptacosanol	13.72	4.0	ng	207469	5	13.88	1034690	20.0
Docosane, 11-butyl-	15.72	10.7	ng	289989	6	15.32	541231	20.0