LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012422\
Data File : BF126652.D
Acq On : 24 Jan 2022 21:11
Operator : CG/JU
Sample : N1242-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PSC-124042

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-BF011822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126652.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.299	29	36	43	rVB	298766	387805	11.54%	1.551%
2	2.551	73	79	88	rBV	18147	35241	1.05%	0.141%
3	3.557	242	250	258	rBV	106066	204750	6.09%	0.819%
4	5.204	523	530	536	rBV	31070	40774	1.21%	0.163%
5	5.581	589	594	597	rBV	3078108	3196173	95.12%	12.785%
6	6.157	689	692	697	rBV	39722	39870	1.19%	0.159%
7	6.575	758	763	767	rBV	2882428	3359980	100.00%	13.440%
8	6.963	825	829	832	rVB	975630	771344	22.96%	3.085%
9	7.522	917	924	927	rBV	2155231	2206062	65.66%	8.824%
10	8.133	1025	1028	1032	rBV	61168	58469	1.74%	0.234%
11	8.245	1043	1047	1050	rBV	1198782	1001305	29.80%	4.005%
12	8.316	1056	1059	1068	rVB	54199	53600	1.60%	0.214%
13	9.322	1225	1230	1233	rBV	3624522	3099018	92.23%	12.396%
14	9.392	1239	1242	1244	rBV	55343	43038	1.28%	0.172%
15	9.798	1308	1311	1316	rVB3	47642	55740	1.66%	0.223%
16	9.922	1326	1332	1335	rBV	44097	40474	1.20%	0.162%
17	10.004	1342	1346	1349	rBV	1396798	1108441	32.99%	4.434%
18	10.033	1349	1351	1354	rVB	78114	61001	1.82%	0.244%
19	10.210	1378	1381	1384	rVB	53564	48796	1.45%	0.195%
20	10.422	1415	1417	1420	rVB2	46838	44072	1.31%	0.176%
21	10.551	1436	1439	1444	rVB	84676	65131	1.94%	0.261%
22	10.792	1476	1480	1484	rBV	2203042	1911107	56.88%	7.645%
23	10.898	1496	1498	1500	rBV2	39630	42546	1.27%	0.170%
24	10.998	1512	1515	1519	rBV2	60602	64100	1.91%	0.256%
25	11.098	1528	1532	1534	rBV4	28163	42193	1.26%	0.169%
26	11.145	1538	1540	1544	rVB4	38390	43262	1.29%	0.173%
27	11.186	1544	1547	1551	rBV	61950	60867	1.81%	0.243%
28	11.351	1568	1575	1577	rBV3	48970	57899	1.72%	0.232%
29	11.380	1577	1580	1585	rVB3	37935	57889	1.72%	0.232%
30	11.439	1588	1590	1596	rVB3	50772	47243	1.41%	0.189%
31	11.498	1596	1600	1602	rBV	1188071	1051646	31.30%	4.207%
32	11.521	1602	1604	1607	rVB	309632	233202	6.94%	0.933%
33	11.651	1624	1626	1632	rBV	41654	48070	1.43%	0.192%
34	12.004	1681	1686	1688	rBV2	80255	100506	2.99%	0.402%
35	12.051	1692	1694	1696	rVB	64061	43686	1.30%	0.175%
36	12.110	1701	1704	1707	rBV2	40009	42570	1.27%	0.170%

LSC Area Percent Report

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Operator : CG/JU
Sample : N1242-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PSC-124042

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-BF011822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.710	1803	1806	1811	rVB	250165	218318	6.50%	0.873%
38	12.939	1839	1845	1850	rBV2	152152	204493	6.09%	0.818%
39	12.986	1850	1853	1858	rVB4	36870	45509	1.35%	0.182%
40	13.086	1866	1870	1873	rVB	2844838	2338993	69.61%	9.356%
41	13.927	2009	2013	2017	rBV4	40046	57699	1.72%	0.231%
42	13.974	2017	2021	2029	rVB2	282987	302621	9.01%	1.211%
43	14.115	2042	2045	2046	rBV	107101	91852	2.73%	0.367%
44	14.139	2046	2049	2052	rVV	734386	741910	22.08%	2.968%
45	14.168	2052	2054	2056	rVB	61244	47909	1.43%	0.192%
46	14.615	2127	2130	2135	rVB4	30303	38355	1.14%	0.153%
47	14.774	2154	2157	2159	rBV	81968	80332	2.39%	0.321%
48	15.209	2228	2231	2235	rBV	44807	69347	2.06%	0.277%
49	15.533	2282	2286	2290	rBV	35230	47293	1.41%	0.189%
50	15.598	2293	2297	2302	rVB	37520	54299	1.62%	0.217%
51	15.668	2304	2309	2320	rBV2	559350	748482	22.28%	2.994%
52	16.168	2391	2394	2399	rVB6	28218	42517	1.27%	0.170%
53	16.221	2399	2403	2411	rBV5	51372	101687	3.03%	0.407%

Sum of corrected areas: 24999486

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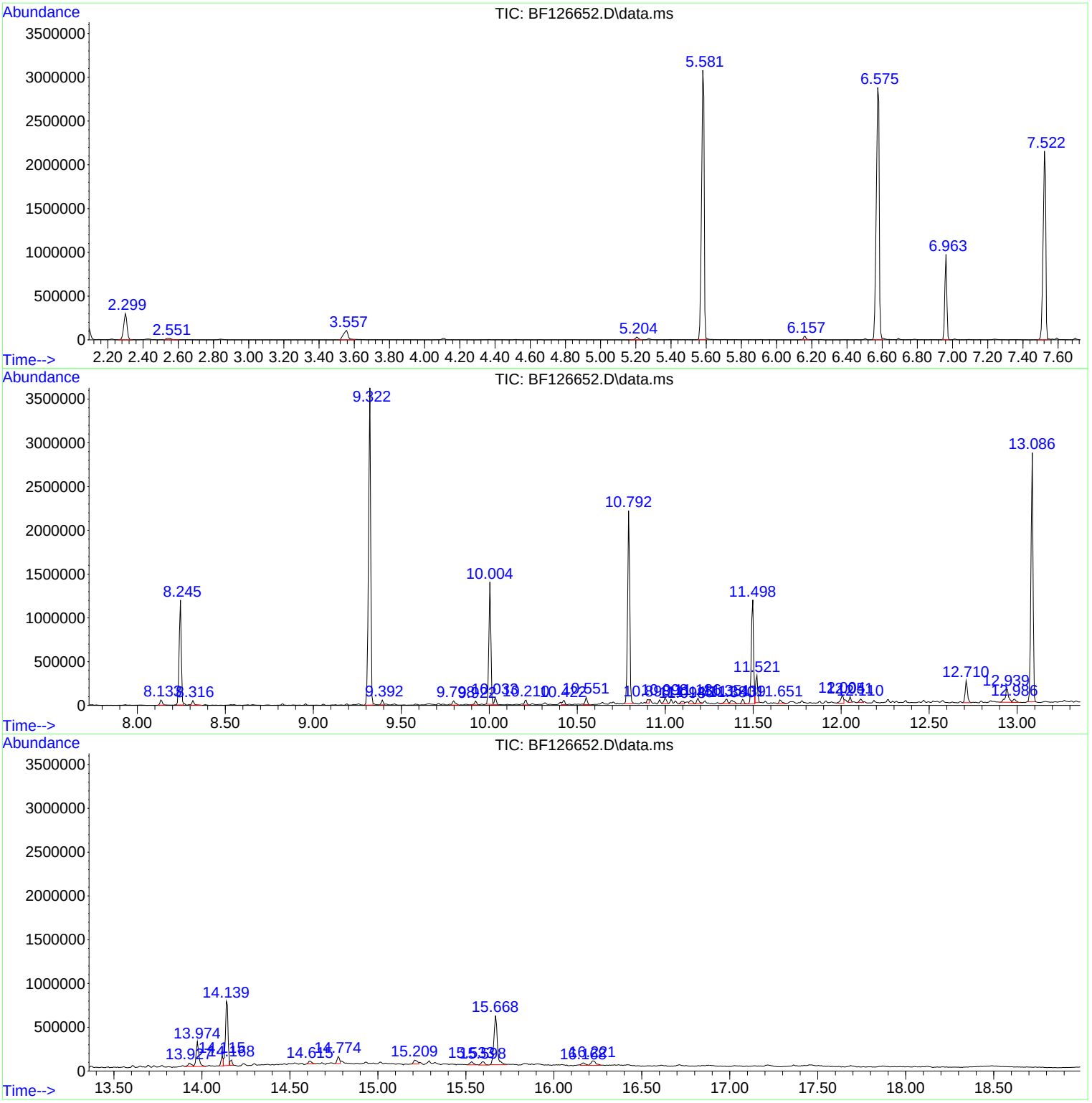
Instrument :
BNA_F
ClientSampleId :
PSC-124042

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012422\
Data File : BF126652.D
Acq On : 24 Jan 2022 21:11
Operator : CG/JU
Sample : N1242-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PSC-124042

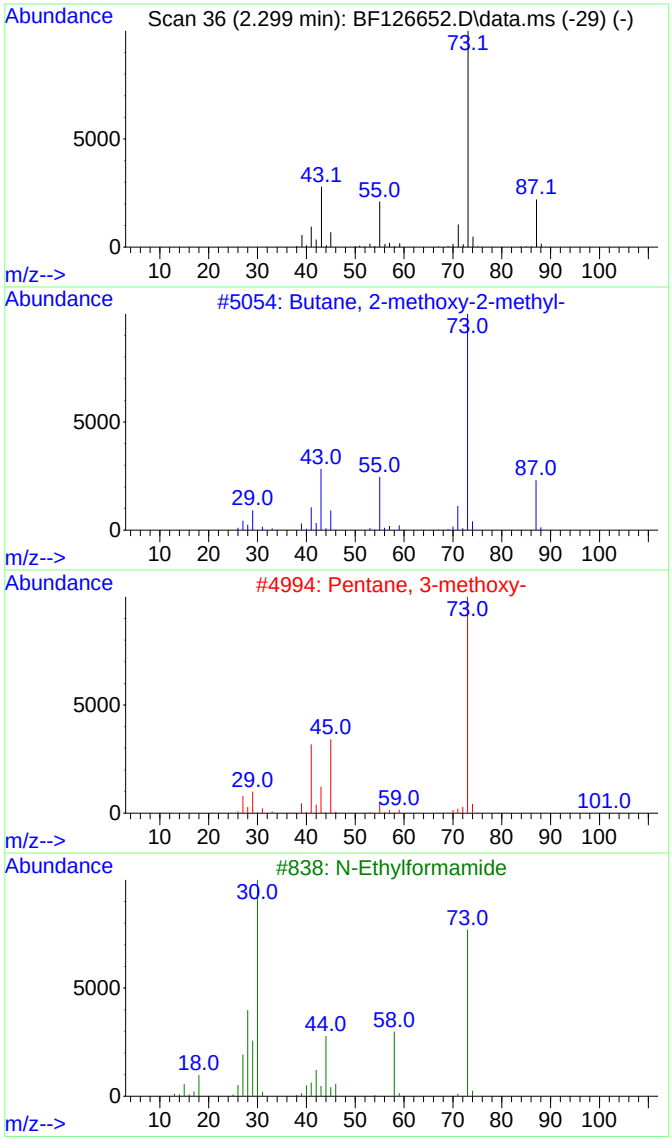
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

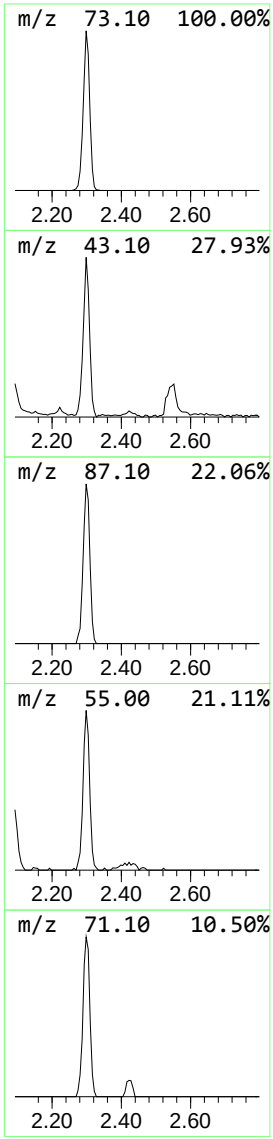
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.299	10.06 ng	387805	1,4-Dichlorobenzene-d4	6.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Data File : BF126652.D
Acq On : 24 Jan 2022 21:11
Operator : CG/JU
Sample : N1242-01
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PSC-124042

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

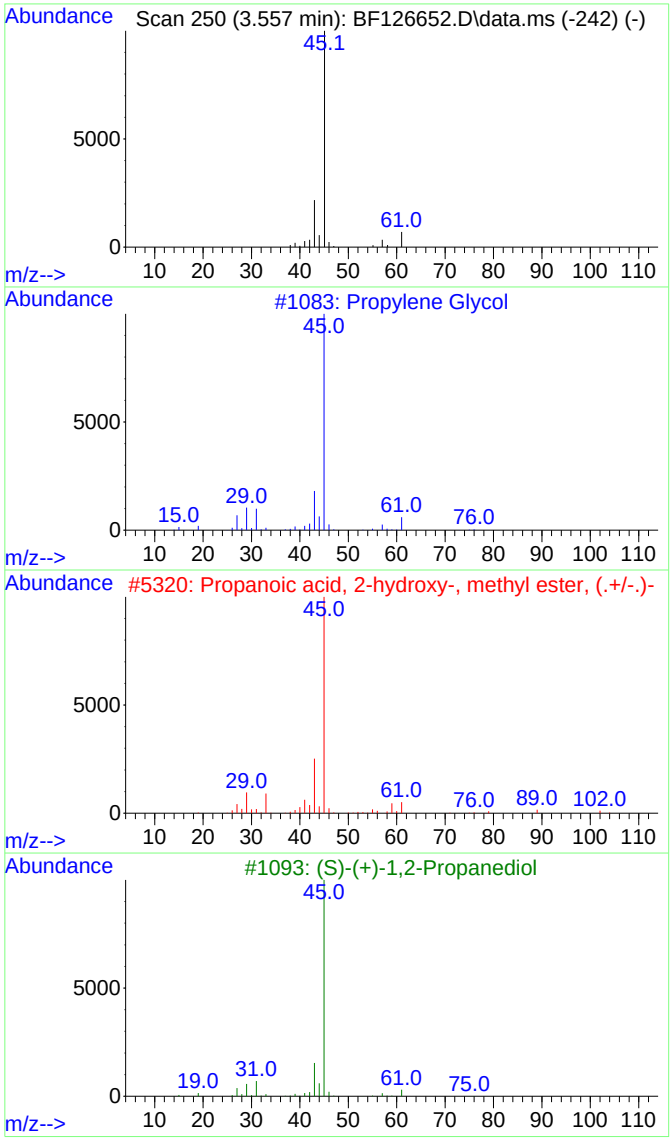
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

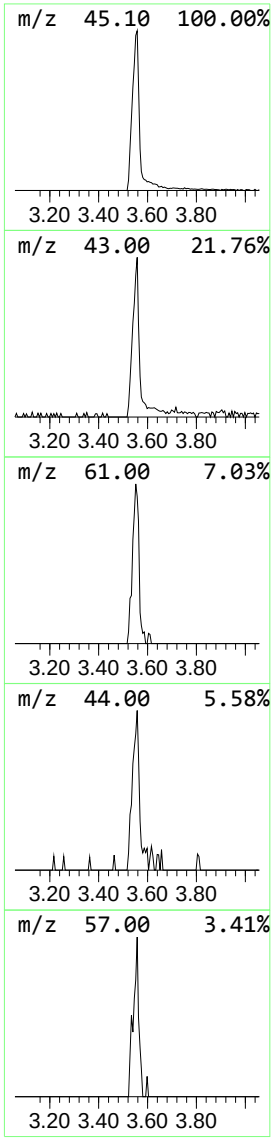
****

Peak Number 2 unknown3.557 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.557	5.31 ng	204750	1,4-Dichlorobenzene-d4	6.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	43
2	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
4	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
5	Isopropyl Alcohol	60	C3H8O	000067-63-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012422\
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

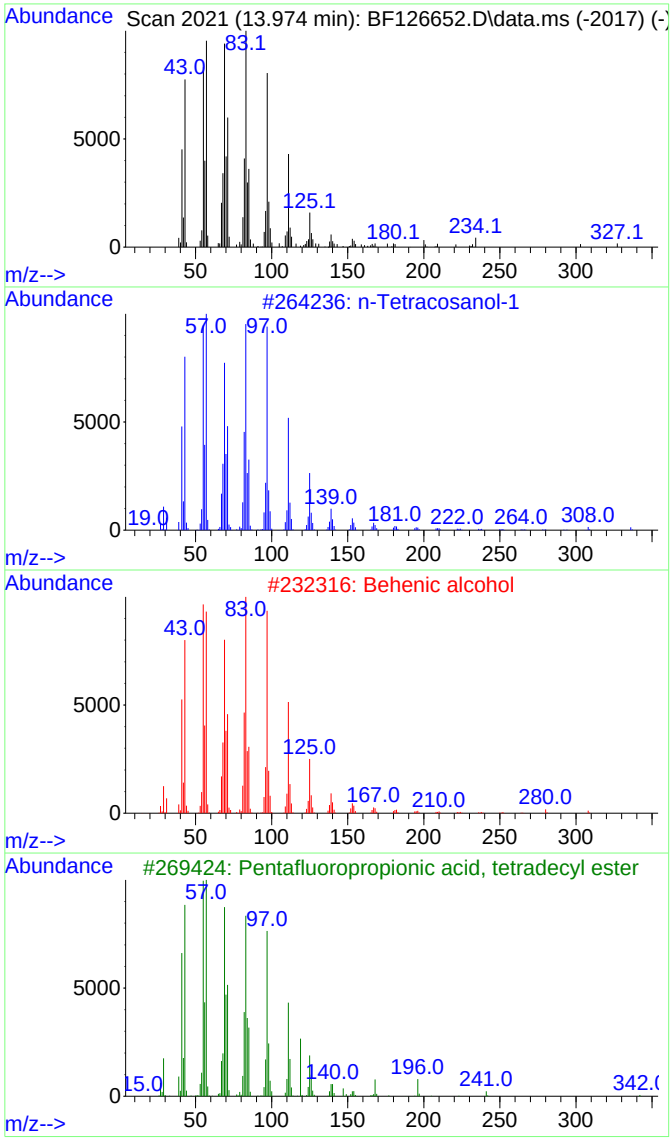
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

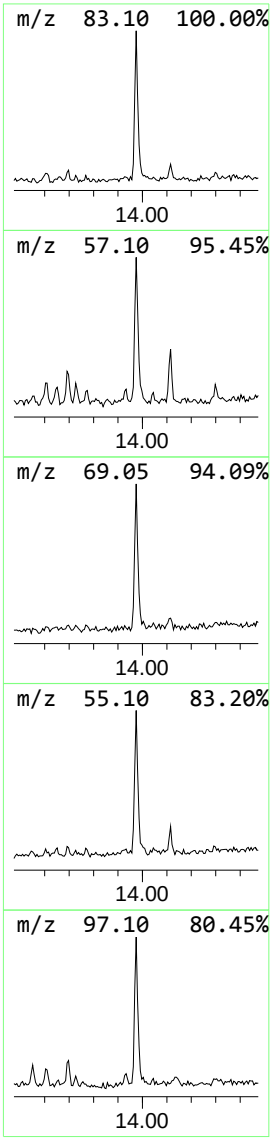
****

Peak Number 3 n-Tetracosanol-1 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.974	8.16 ng	302621	Chrysene-d12	14.145

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2	Behenic alcohol	326	C22H46O	000661-19-8	91
3	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91
4	1-Hexacosanol	382	C26H54O	000506-52-5	91
5	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012422\
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Sample : N1242-01
Misc :
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Instrument :
BNA_F
ClientSampleId :
PSC-124042

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

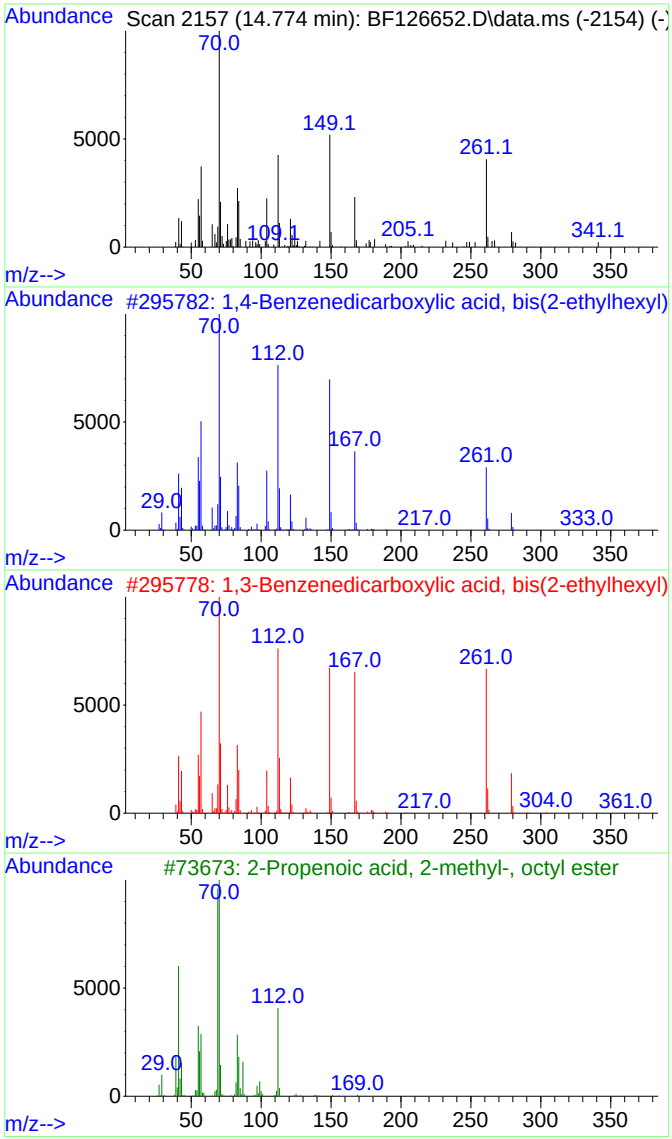
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

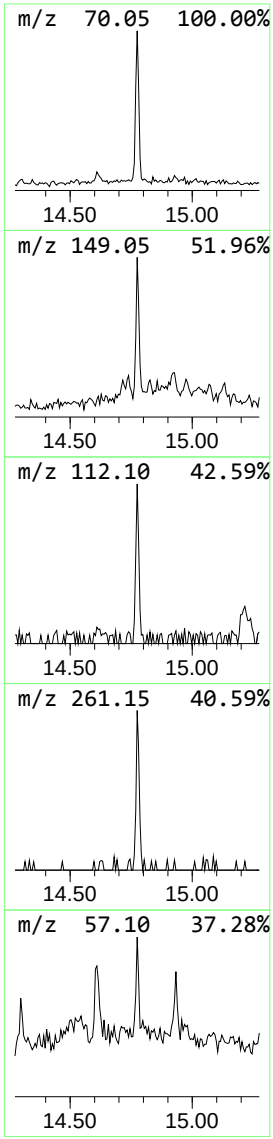
****

Peak Number 4 unknown14.774 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.774	2.17 ng	80332	Chrysene-d12	14.145

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	49
2	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	47
3	2-Propenoic acid, 2-methyl-, oct...	198	C12H22O2	002157-01-9	32
4	(E)-Tetradec-2-enal	210	C14H26O	051534-36-2	16
5	5-Undecene, 3-methyl-, (E)-	168	C12H24	074630-67-4	14





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Instrument :
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ClientSampleId :
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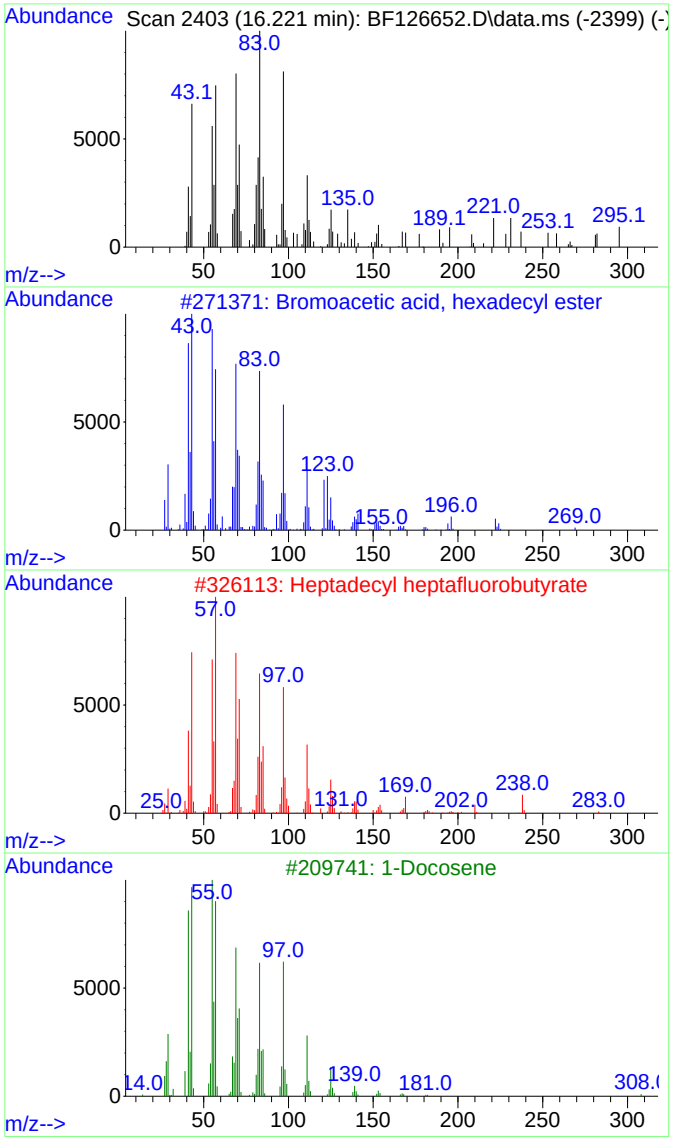
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

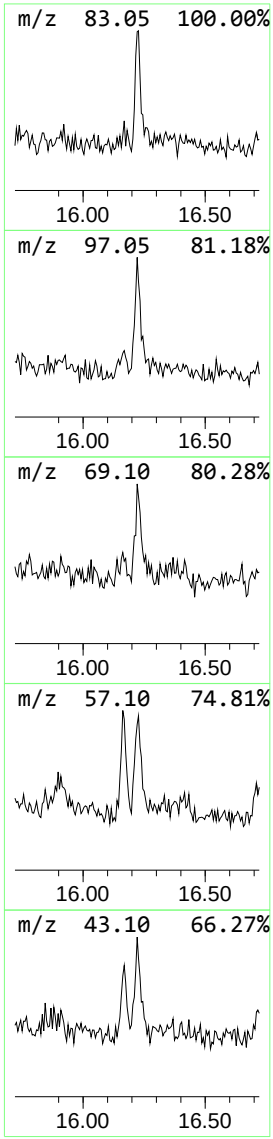
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Bromoacetic acid, hexadecyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.221	2.72 ng	101687	Perylene-d12	15.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	90
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	58
3	1-Docosene	308	C22H44	001599-67-3	58
4	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	49
5	1-Dotriacontanol, acetate	509	C34H68O2	023811-94-1	45





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012422\
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.299	10.1	ng	387805	1	6.963	771344	20.0
unknown3.557	3.557	5.3	ng	204750	1	6.963	771344	20.0
n-Tetracosanol-1	13.974	8.2	ng	302621	5	14.145	741910	20.0
unknown14.774	14.774	2.2	ng	80332	5	14.145	741910	20.0
Bromoacetic aci...	16.221	2.7	ng	101687	6	15.668	748482	20.0