LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
Data File : BF103774.D
Acq On : 19 Mar 2018 23:38
Operator : JU/SJ
Sample : J1972-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2 COMP

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-BF031518.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	2.322	34	40	47	rVB	159823	216858	5.64%	0.573%
2	5.222	529	533	541	rVB	165987	223182	5.81%	0.590%
3	5.598	592	597	600	rBV	3424714	3787356	98.51%	10.004%
4	5.922	648	652	657	rBV	48617	47751	1.24%	0.126%
5	6.598	760	767	770	rBV	3310540	3818196	99.31%	10.086%
6	6.745	787	792	795	rBV	3768542	3799243	98.82%	10.036%
7	6.975	827	831	834	rVB	951128	830141	21.59%	2.193%
8	7.128	853	857	861	rBV	3000518	3007096	78.22%	7.943%
9	7.534	921	926	929	rBV	2336269	2449608	63.72%	6.471%
10	7.598	932	937	946	rVB	41217	46959	1.22%	0.124%
11	8.251	1044	1048	1052	rBV	1229472	1088687	28.32%	2.876%
12	9.328	1226	1231	1234	rBV	3993714	3844632	100.00%	10.156%
13	9.716	1293	1297	1300	rBV	555732	417040	10.85%	1.102%
14	9.928	1329	1333	1336	rVB	95652	71141	1.85%	0.188%
15	10.016	1343	1348	1351	rBV	1182046	1136708	29.57%	3.003%
16	10.427	1416	1418	1421	rVB	119278	86454	2.25%	0.228%
17	10.651	1450	1456	1458	rBV	34007	43874	1.14%	0.116%
18	10.710	1461	1466	1469	rBV2	44343	49309	1.28%	0.130%
19	10.804	1478	1482	1486	rBV	2273830	2298615	59.79%	6.072%
20	10.904	1496	1499	1505	rVB	96185	100837	2.62%	0.266%
21	11.351	1571	1575	1578	rBV	65154	52619	1.37%	0.139%
22	11.504	1597	1601	1603	rBV	1256685	1038893	27.02%	2.744%
23	11.527	1603	1605	1610	rVB	352371	278965	7.26%	0.737%
24	11.580	1610	1614	1617	rBV	75963	60891	1.58%	0.161%
25	12.016	1684	1688	1690	rBV2	148381	170949	4.45%	0.452%
26	12.033	1690	1691	1696	rVB2	77298	53049	1.38%	0.140%
27	12.121	1702	1706	1708	rBV2	67133	72862	1.90%	0.192%
28	12.721	1804	1808	1812	rBV	572692	469376	12.21%	1.240%
29	12.951	1841	1847	1853	rBV	426456	501754	13.05%	1.325%
30	13.092	1864	1871	1875	rBV	3047657	3091994	80.42%	8.168%
31	13.163	1880	1883	1888	rVB2	27040	41983	1.09%	0.111%
32	13.280	1900	1903	1906	rVB2	81977	78734	2.05%	0.208%
33	13.345	1911	1914	1917	rBV	51803	41923	1.09%	0.111%
34	13.386	1917	1921	1924	rBV2	37732	43427	1.13%	0.115%

LSC Area Percent Report

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Instrument : BNA_F
ClientSampleId : S-2 COMP

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-BF031518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.904	2003	2009	2012	rBV2	50725	77994	2.03%	0.206%
36	13.974	2016	2021	2030	rVB4	518273	584235	15.20%	1.543%
37	14.157	2047	2052	2055	rBV2	1068563	1175985	30.59%	3.106%
38	14.180	2055	2056	2062	rVB	250245	182571	4.75%	0.482%
39	14.263	2064	2070	2072	rBV3	47037	68922	1.79%	0.182%
40	14.298	2073	2076	2081	rBV4	39849	46358	1.21%	0.122%
41	14.621	2127	2131	2134	rBV2	88391	117680	3.06%	0.311%
42	15.233	2231	2235	2239	rBV	186620	303681	7.90%	0.802%
43	15.321	2247	2250	2253	rBV	47481	45458	1.18%	0.120%
44	15.557	2287	2290	2297	rVB	112312	163941	4.26%	0.433%
45	15.621	2297	2301	2308	rVB	149364	209824	5.46%	0.554%
46	15.698	2308	2314	2318	rBV	588830	816115	21.23%	2.156%
47	16.221	2399	2403	2412	rVB4	86018	160055	4.16%	0.423%
48	17.262	2575	2580	2589	rVB3	80548	175659	4.57%	0.464%
49	17.445	2607	2611	2619	rVB6	31765	64167	1.67%	0.169%
50	17.739	2656	2661	2671	rVB2	57805	127874	3.33%	0.338%
51	17.886	2681	2686	2698	rVB2	69713	175619	4.57%	0.464%

Sum of corrected areas: 37857244

LSC Report - Integrated Chromatogram

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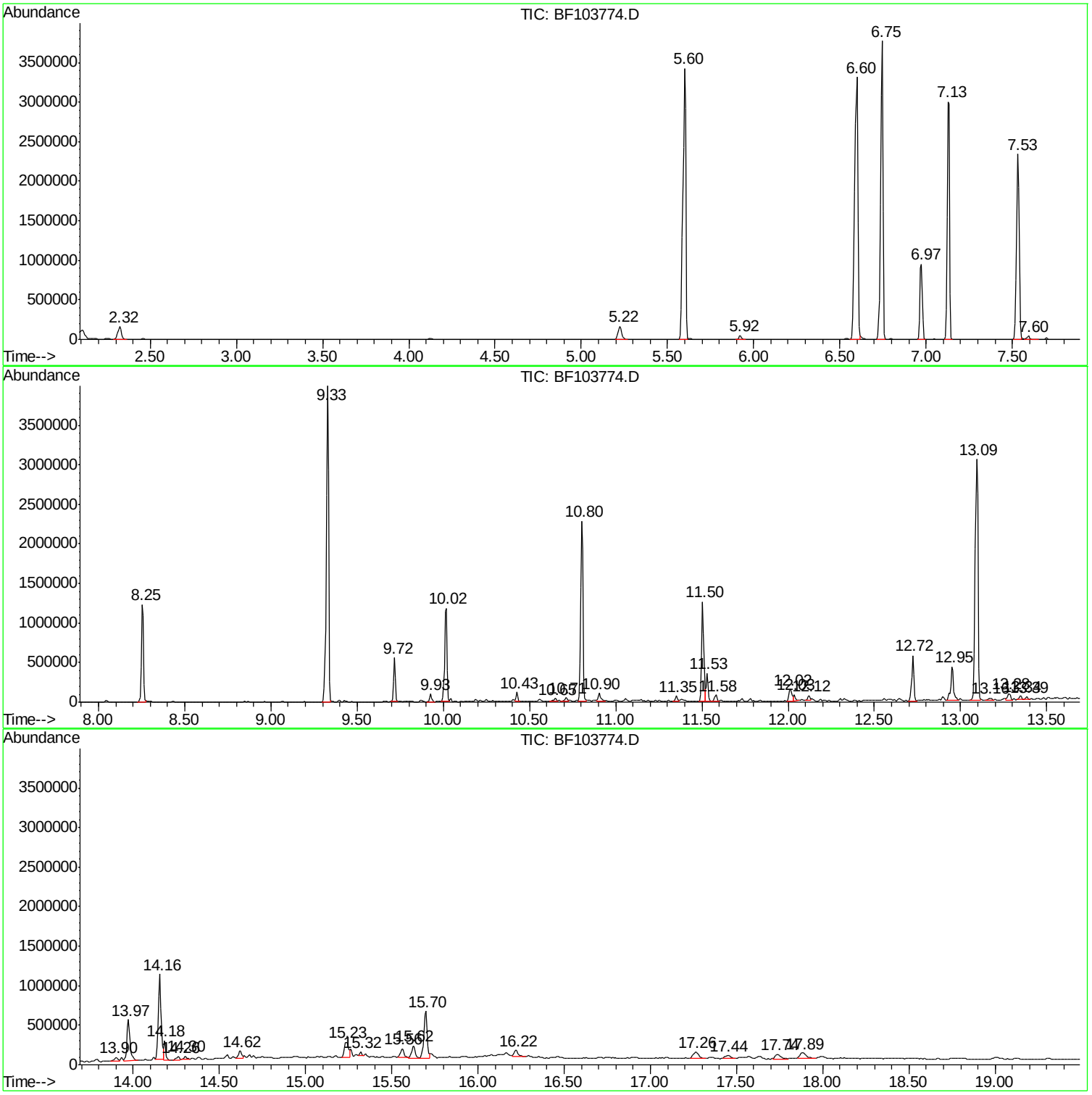
Operator : JU/SJ
Sample : J1972-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2 COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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\BF031918\
Data File : BF103774.D
Acq On : 19 Mar 2018 23:38
Operator : JU/SJ
Sample : J1972-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2 COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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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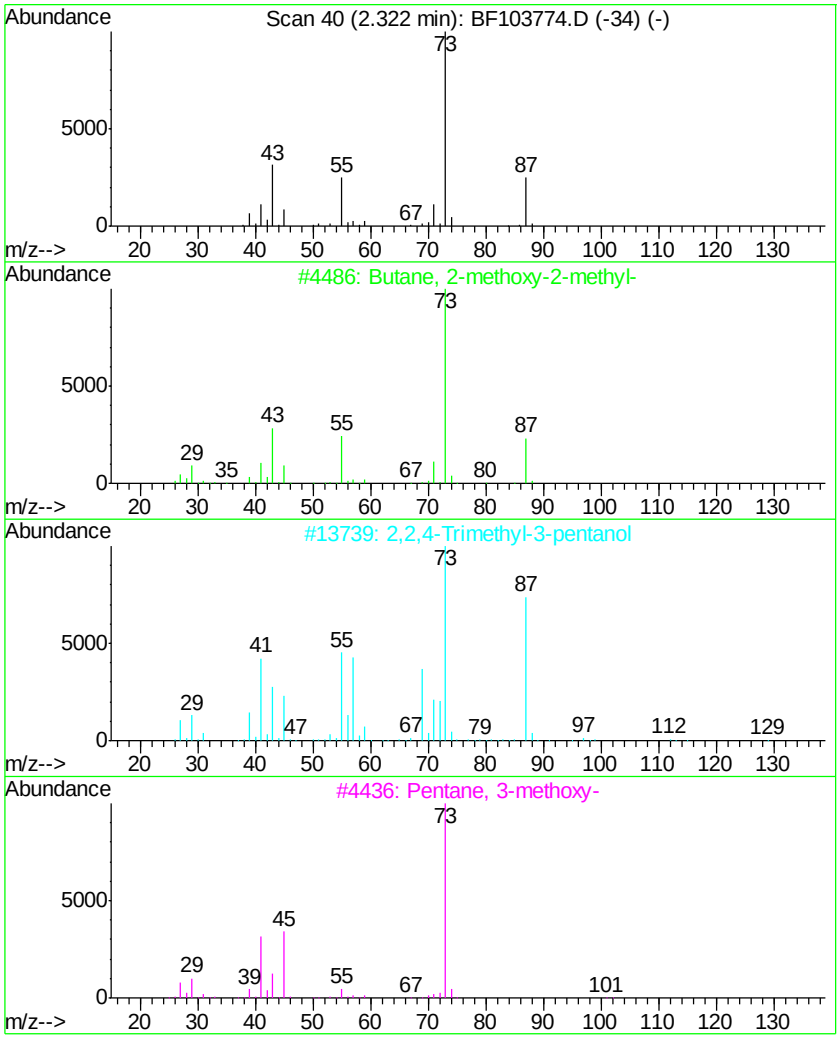
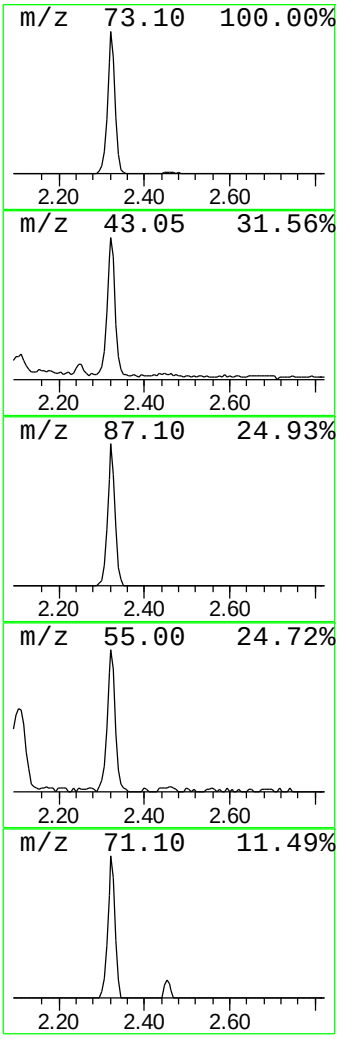
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.32	5.22 ng	216858	1,4-Dichlorobenzene-d4	6.97

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	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Sample : J1972-04
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ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2 COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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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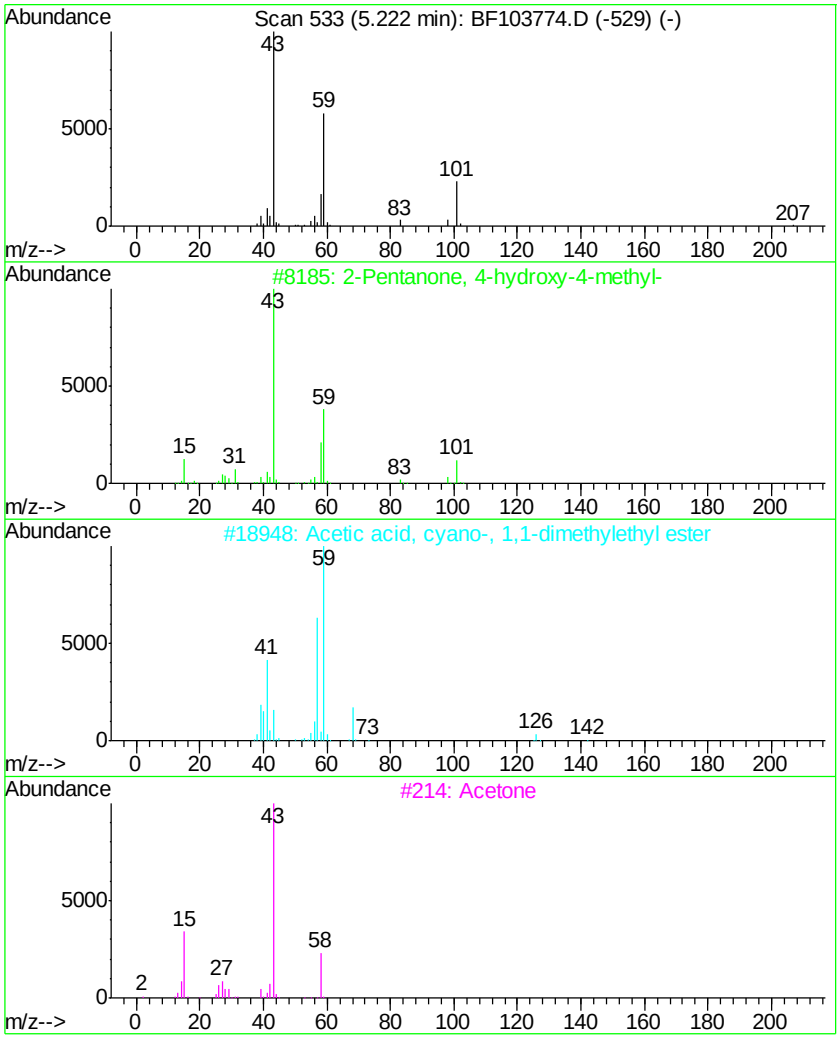
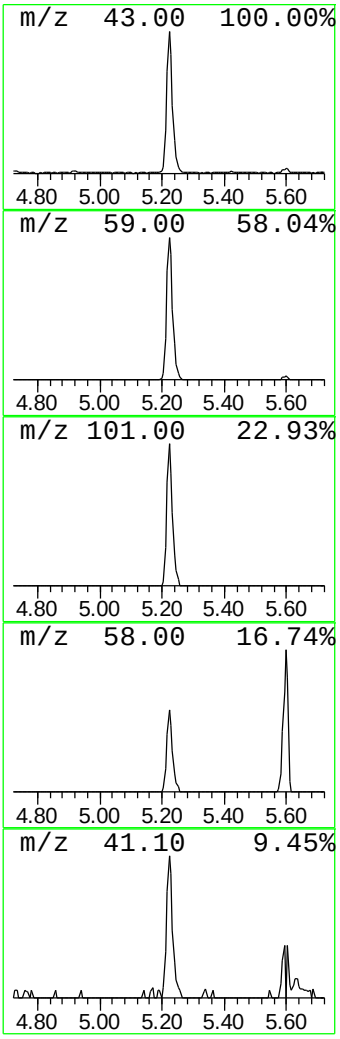
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	5.38 ng	223182	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Acetone	58	C3H6O	000067-64-1	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Propanoic acid, 2-hydroxy-2-meth...	132	C6H12O3	000080-55-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
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Operator : JU/SJ
Sample : J1972-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2 COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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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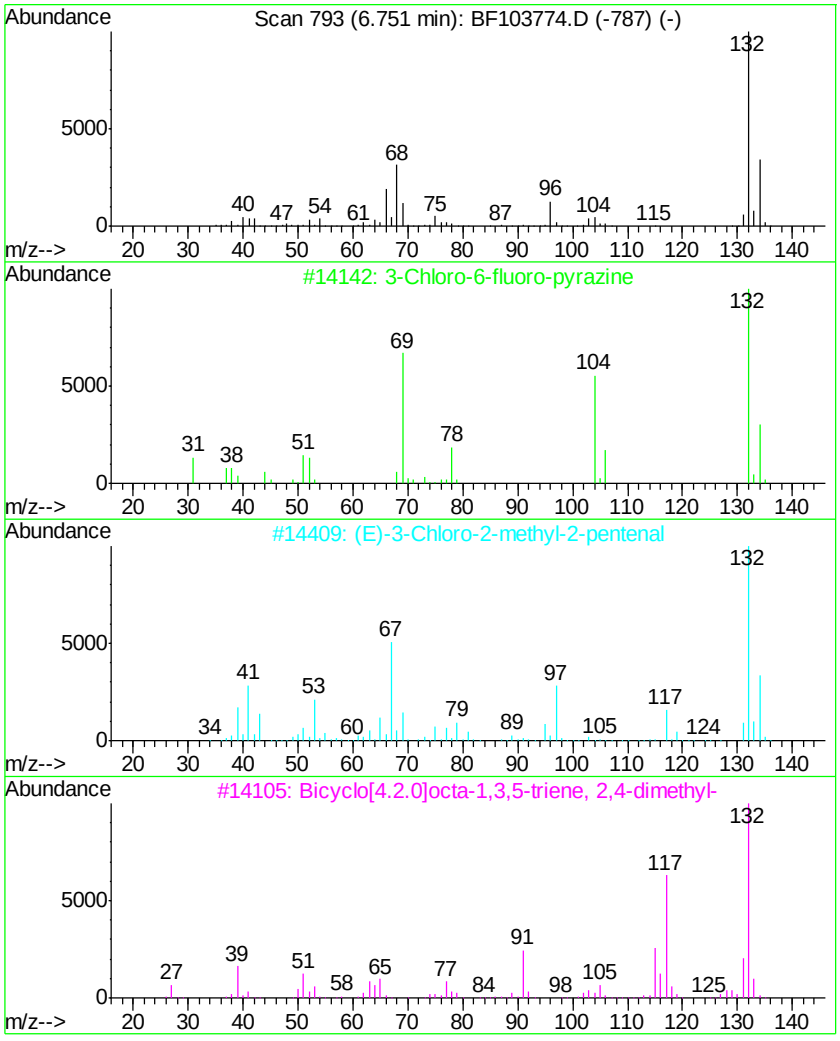
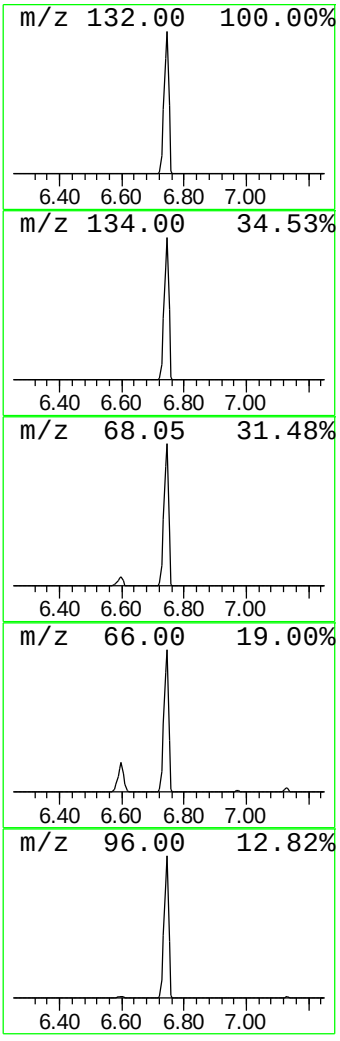
Peak Number 3 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	91.53 ng	3799240	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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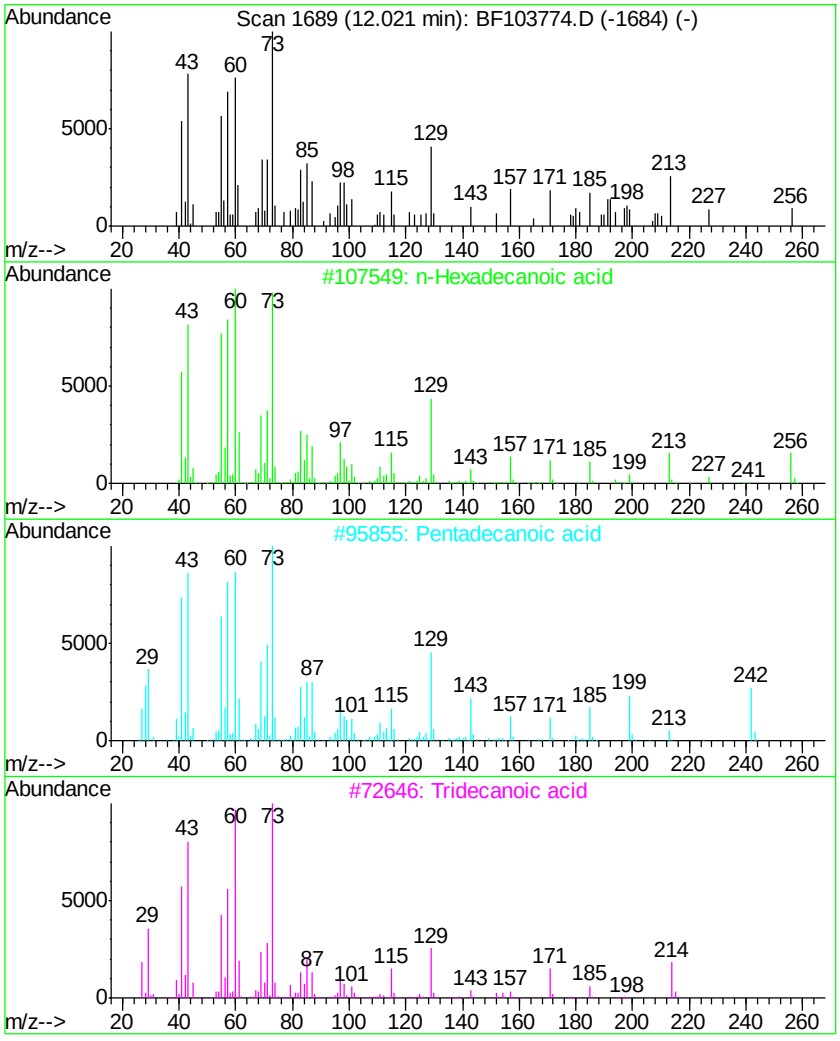
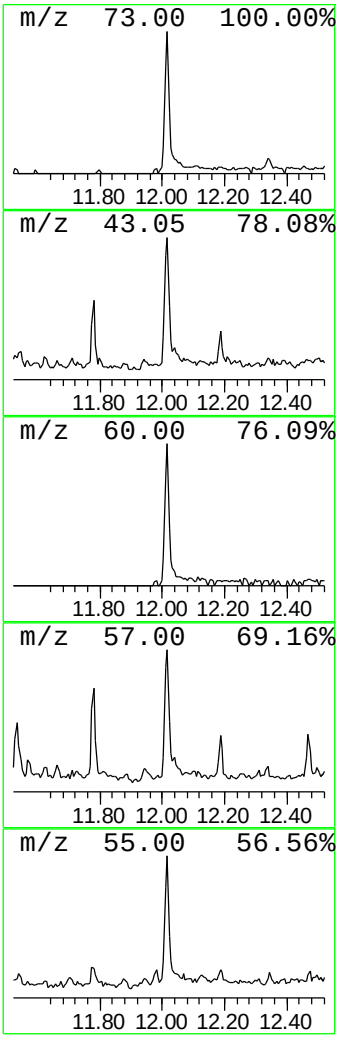
Peak Number 5 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	3.29 ng	170949	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Tetradecane	198	C14H30	000629-59-4	53
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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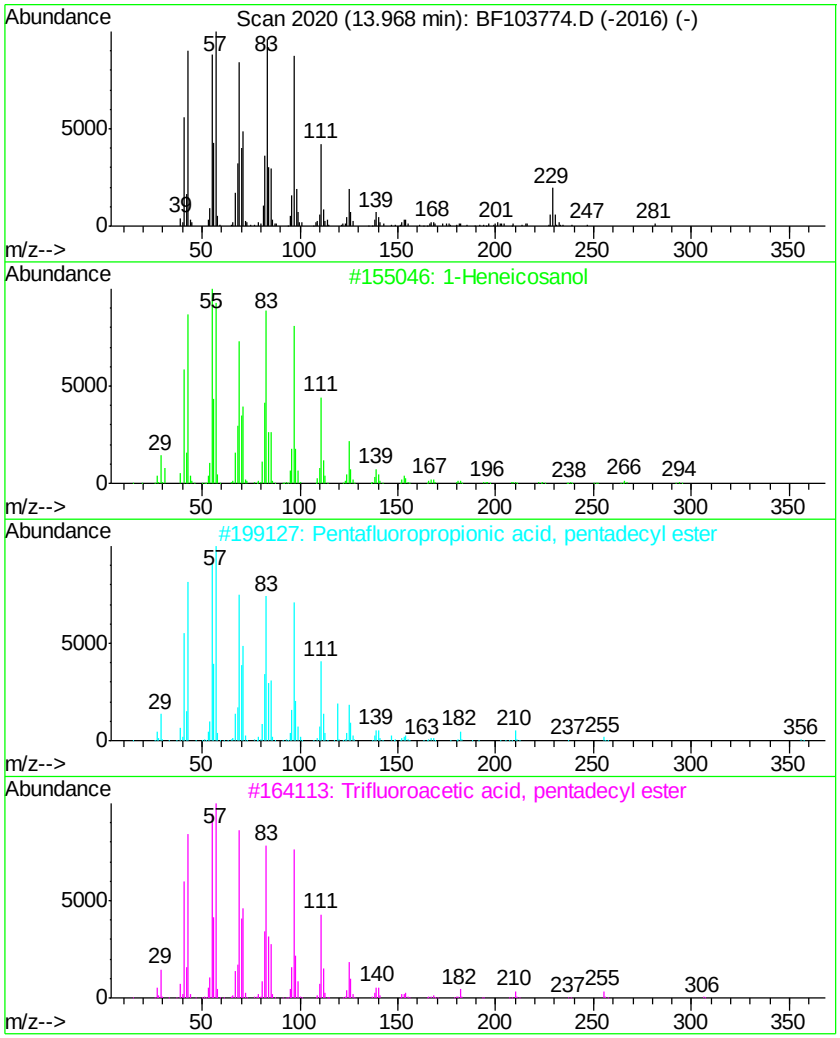
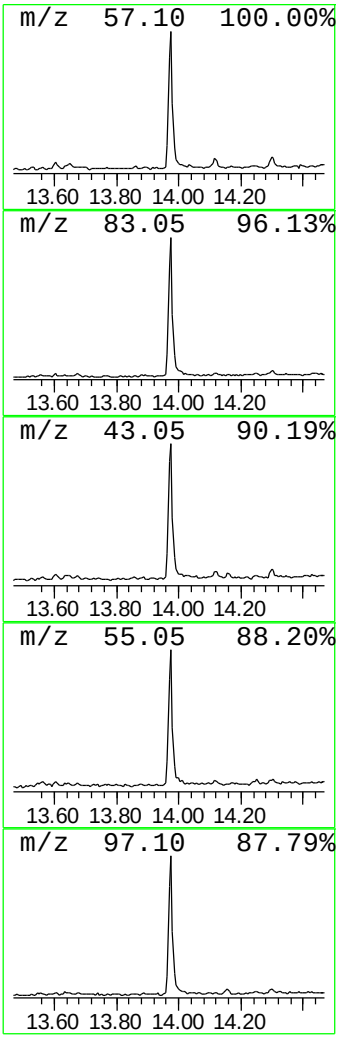
Peak Number 6 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	9.94 ng	584235	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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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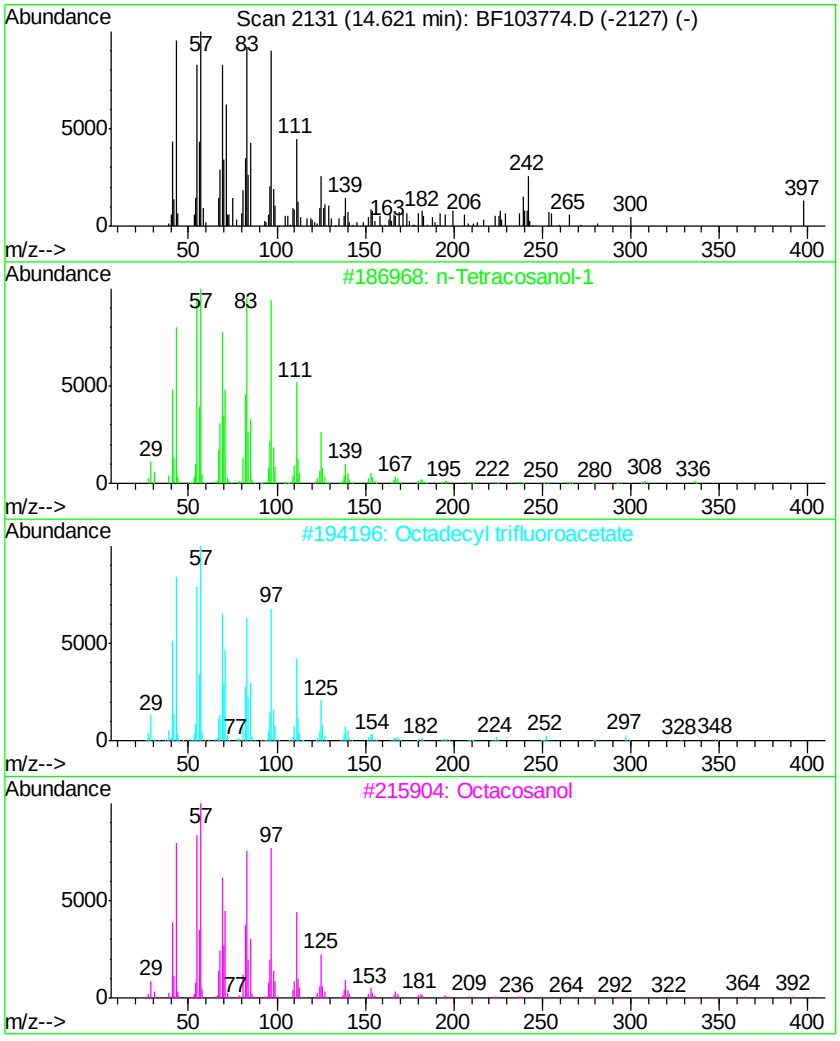
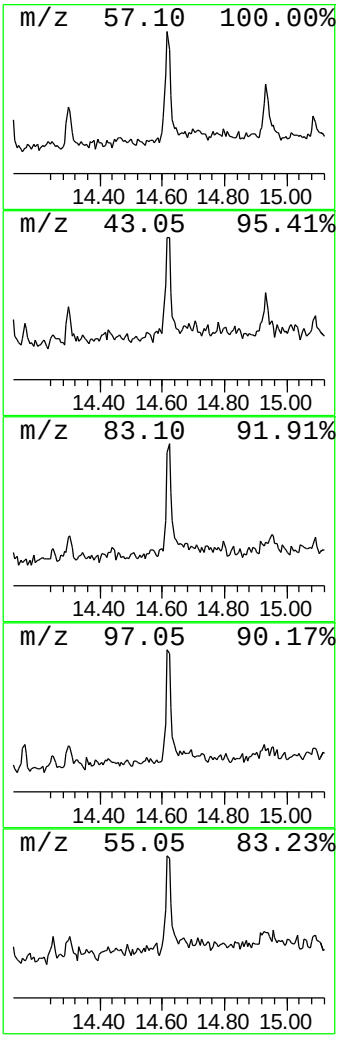
Peak Number 7 n-Tetracosanol-1 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	2.00 ng	117680	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
2	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	93
3	Octacosanol	410	C28H58O	000557-61-9	93
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	93





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Instrument : BNA_F
ClientSampleId : S-2 COMP

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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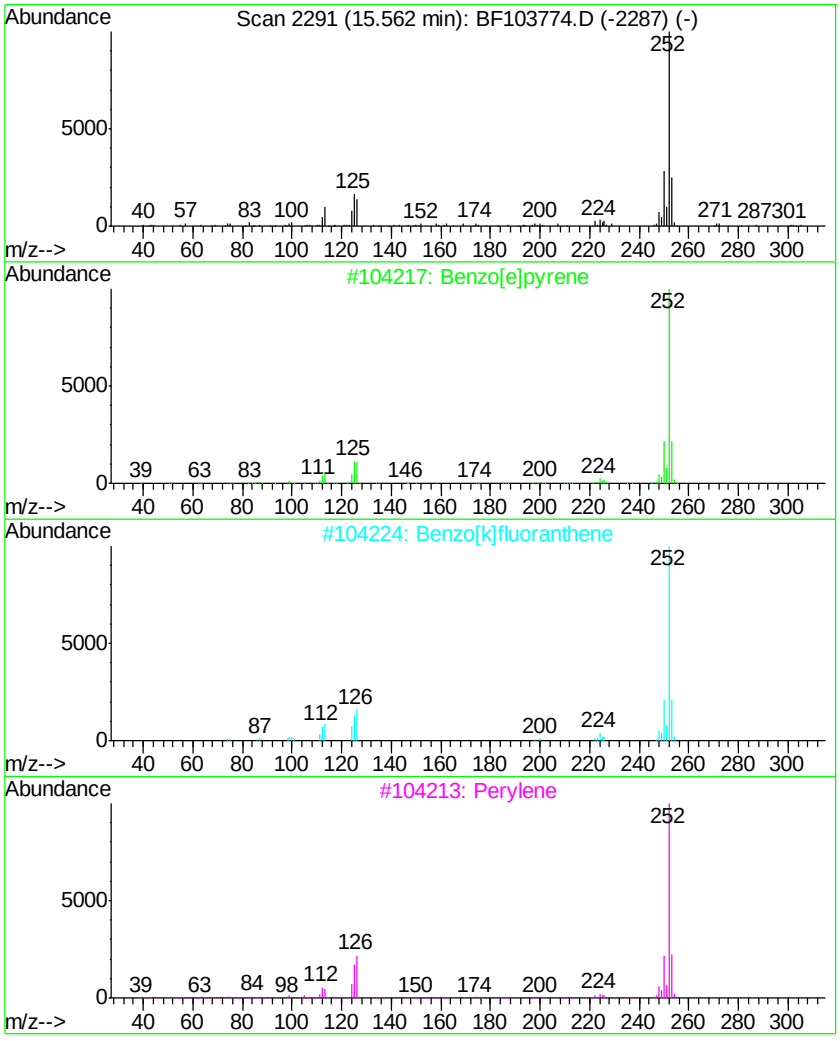
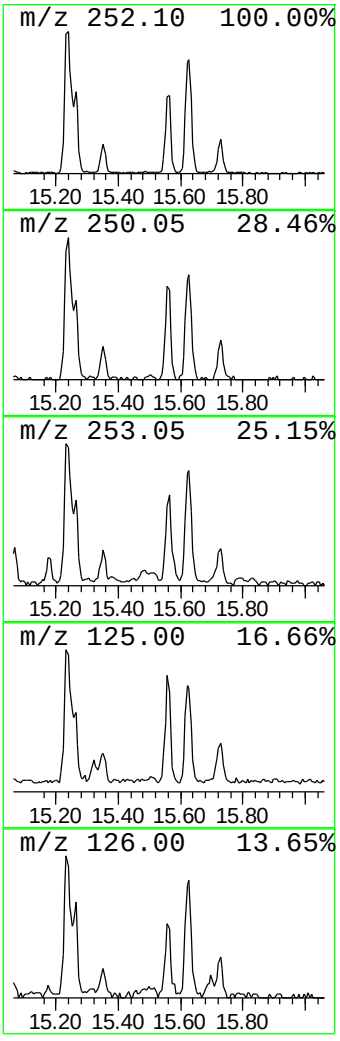
Peak Number 8 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.56	4.02 ng	163941	Perylene-d12	15.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
3	Perylene	252	C20H12	000198-55-0	96
4	Benzo[a]pyrene	252	C20H12	000050-32-8	95
5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
Data File : BF103774.D
Acq On : 19 Mar 2018 23:38
Operator : JU/SJ
Sample : J1972-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2 COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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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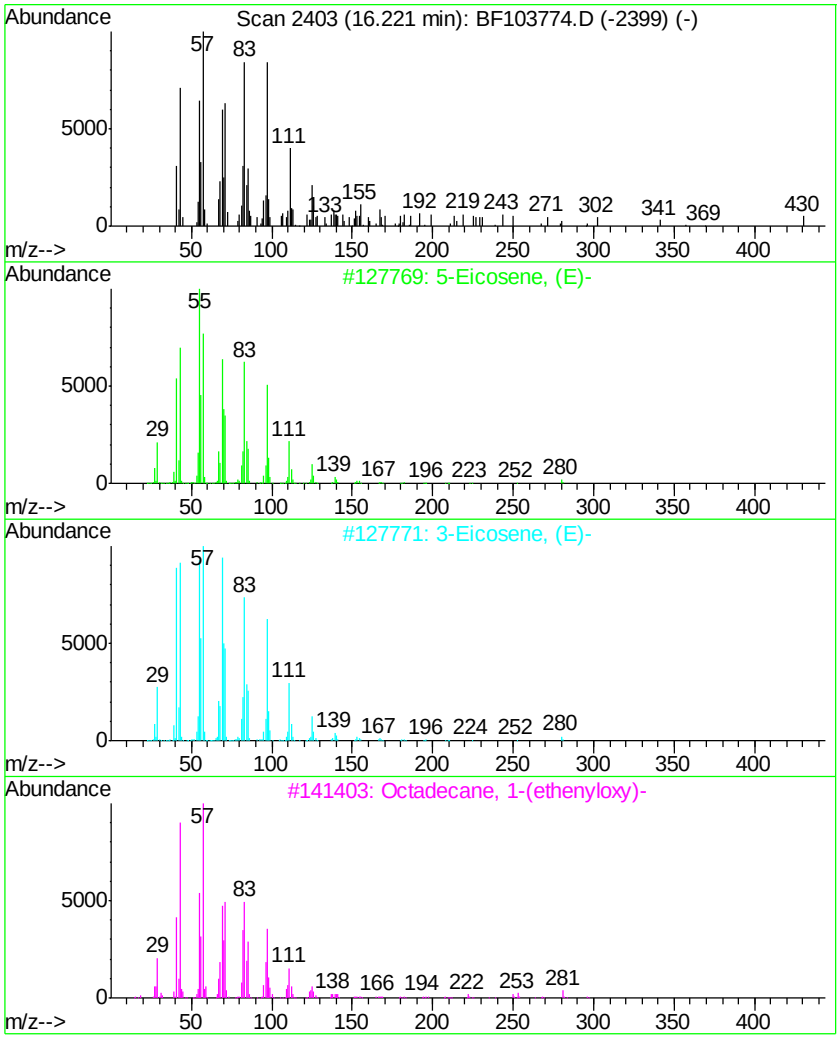
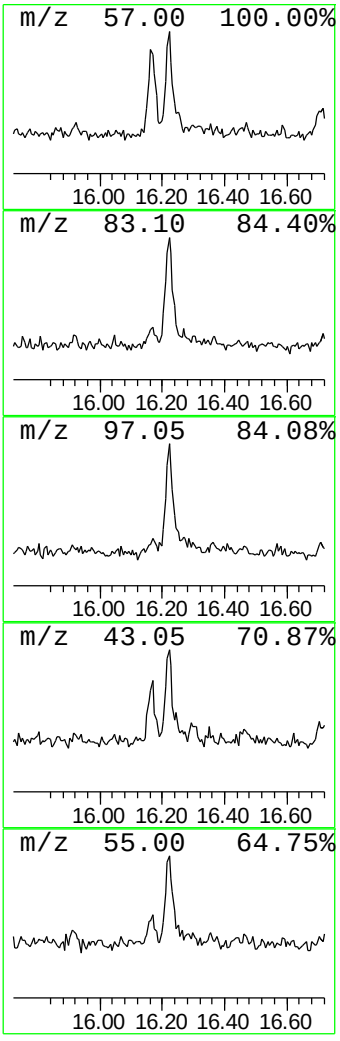
Peak Number 9 5-Eicosene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.22	3.92 ng	160055	Perylene-d12	15.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	93
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	90
4	Behenic alcohol	326	C22H46O	000661-19-8	87
5	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	76





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
Data File : BF103774.D
Acq On : 19 Mar 2018 23:38
Operator : JU/SJ
Sample : J1972-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2 COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

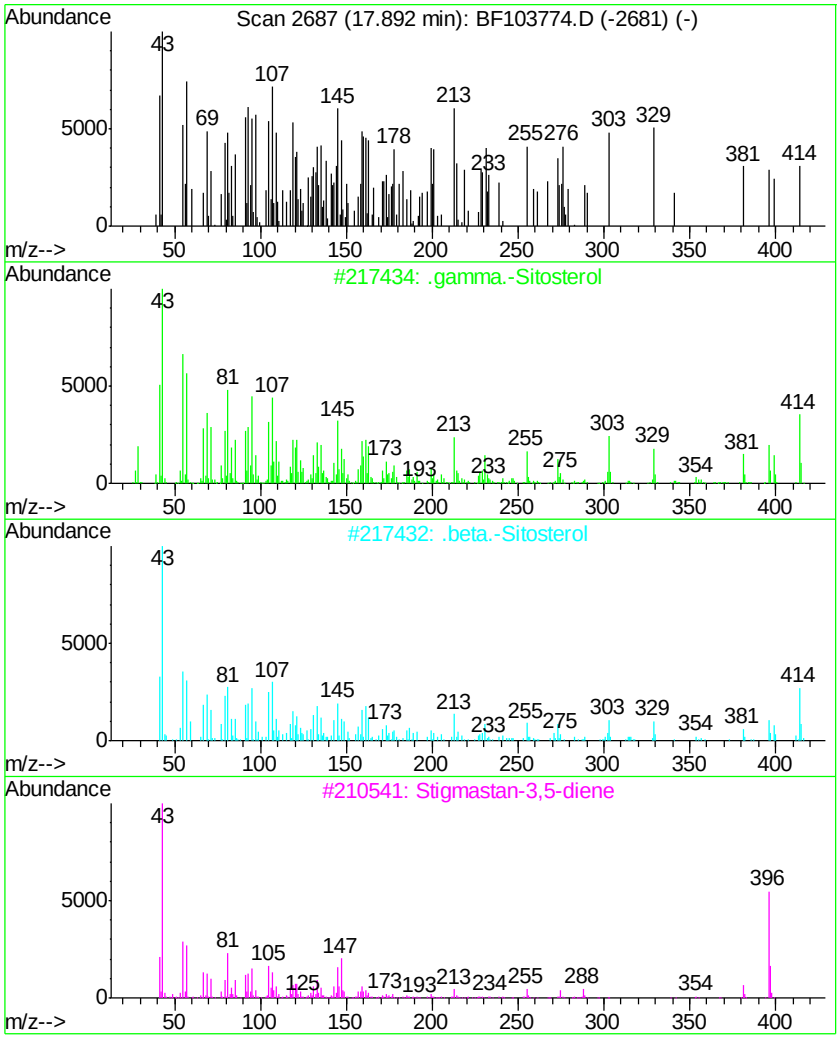
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

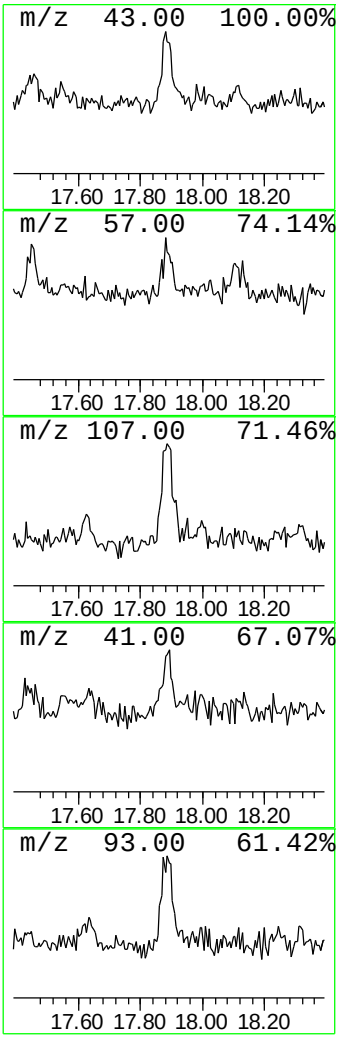
****

Peak Number 10 .gamma.-Sitosterol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.89	4.30 ng	175619	Perylene-d12	15.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	45
3	Stigmastan-3,5-diene	396	C29H48	1000214-16-4	38
4	17-(1,5-Dimethylhexyl)-10,13-dim...	414	C29H50O	1000210-86-9	30
5	Pregn-5-ene-3,12,14,17,20-pentol...	366	C21H34O5	028417-32-5	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031918\
Data File : BF103774.D
Acq On : 19 Mar 2018 23:38
Operator : JU/SJ
Sample : J1972-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2 COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
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...	2.32	5.2	ng	216858	1	6.97	830141	20.0
2-Pentanone, 4-hy...	5.22	5.4	ng	223182	1	6.97	830141	20.0
unknown6.75	6.75	91.5	ng	3799240	1	6.97	830141	20.0
n-Hexadecanoic acid	12.02	3.3	ng	170949	4	11.50	1038890	20.0
1-Heneicosanol	13.97	9.9	ng	584235	5	14.16	1175990	20.0
n-Tetracosanol-1	14.62	2.0	ng	117680	5	14.16	1175990	20.0
Benzo[e]pyrene	15.56	4.0	ng	163941	6	15.70	816115	20.0
5-Eicosene, (E)-	16.22	3.9	ng	160055	6	15.70	816115	20.0
.gamma.-Sitosterol	17.89	4.3	ng	175619	6	15.70	816115	20.0