LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040822\
Data File : BF127714.D
Acq On : 08 Apr 2022 15:29
Operator : CG\JU
Sample : N2317-17
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP1-A

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-BF040622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127714.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.340	3	9	16	rVB	372968	479766	12.15%	1.650%
2	5.210	489	497	506	rVB	224824	294443	7.46%	1.013%
3	5.587	555	561	564	rBV	3357827	3372369	85.41%	11.600%
4	6.581	723	730	733	rBV	3137957	3499798	88.63%	12.038%
5	6.963	791	795	798	rBV	983338	765049	19.38%	2.632%
6	7.528	885	891	894	rBV	2349285	2340780	59.28%	8.052%
7	8.245	1009	1013	1017	rBV	1182735	1016162	25.73%	3.495%
8	9.198	1171	1175	1179	rBV2	53716	50486	1.28%	0.174%
9	9.328	1191	1197	1200	rBV	4139606	3948618	100.00%	13.582%
10	9.381	1203	1206	1212	rVB2	92840	115939	2.94%	0.399%
11	9.663	1251	1254	1257	rBV2	60304	47779	1.21%	0.164%
12	9.704	1257	1261	1264	rVB	85719	73141	1.85%	0.252%
13	9.916	1292	1297	1300	rBV	105757	96933	2.45%	0.333%
14	9.981	1303	1308	1309	rBV	39330	39945	1.01%	0.137%
15	10.010	1309	1313	1315	rVV	1414400	1220089	30.90%	4.197%
16	10.028	1315	1316	1323	rVB2	121297	90265	2.29%	0.310%
17	10.122	1329	1332	1335	rBV	127587	101828	2.58%	0.350%
18	10.163	1335	1339	1342	rVV2	119821	120535	3.05%	0.415%
19	10.216	1342	1348	1355	rVB2	41591	43545	1.10%	0.150%
20	10.798	1439	1447	1451	rBV	3009226	2915583	73.84%	10.029%
21	11.504	1563	1567	1569	rBV	1354042	1218237	30.85%	4.190%
22	11.522	1569	1570	1573	rVB	123012	85403	2.16%	0.294%
23	12.016	1646	1654	1660	rBV3	85078	109113	2.76%	0.375%
24	12.175	1676	1681	1689	rVB3	69653	92604	2.35%	0.319%
25	12.716	1770	1773	1779	rBV	103715	124483	3.15%	0.428%
26	12.945	1807	1812	1816	rVB2	52092	53784	1.36%	0.185%
27	13.092	1833	1837	1840	rBV	3904452	3672293	93.00%	12.632%
28	13.316	1869	1875	1880	rBV3	27259	44390	1.12%	0.153%
29	13.851	1962	1966	1970	rBV	103013	88653	2.25%	0.305%
30	13.992	1986	1990	2004	rBV	182844	403161	10.21%	1.387%
31	14.151	2013	2017	2020	rBV	971936	835626	21.16%	2.874%
32	14.633	2092	2099	2110	rBV2	125495	284063	7.19%	0.977%
33	15.298	2208	2212	2217	rBV	70503	77685	1.97%	0.267%
34	15.357	2217	2222	2230	rBV9	21925	58629	1.48%	0.202%
35	15.674	2271	2276	2286	rBV2	519307	685132	17.35%	2.357%
36	16.180	2356	2362	2368	rBV	41307	64757	1.64%	0.223%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040822\
Data File : BF127714.D
Acq On : 08 Apr 2022 15:29
Operator : CG\JU
Sample : N2317-17
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-A

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-BF040622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.045	2504	2509	2518	rVB	18513	41825	1.06%	0.144%
38	17.910	2648	2656	2663	rBV10	43610	125404	3.18%	0.431%
39	18.274	2711	2718	2723	rBV8	27990	75521	1.91%	0.260%
40	18.498	2749	2756	2767	rVB8	39774	108728	2.75%	0.374%
41	18.792	2797	2806	2820	rBV8	50715	189280	4.79%	0.651%

Sum of corrected areas: 29071824

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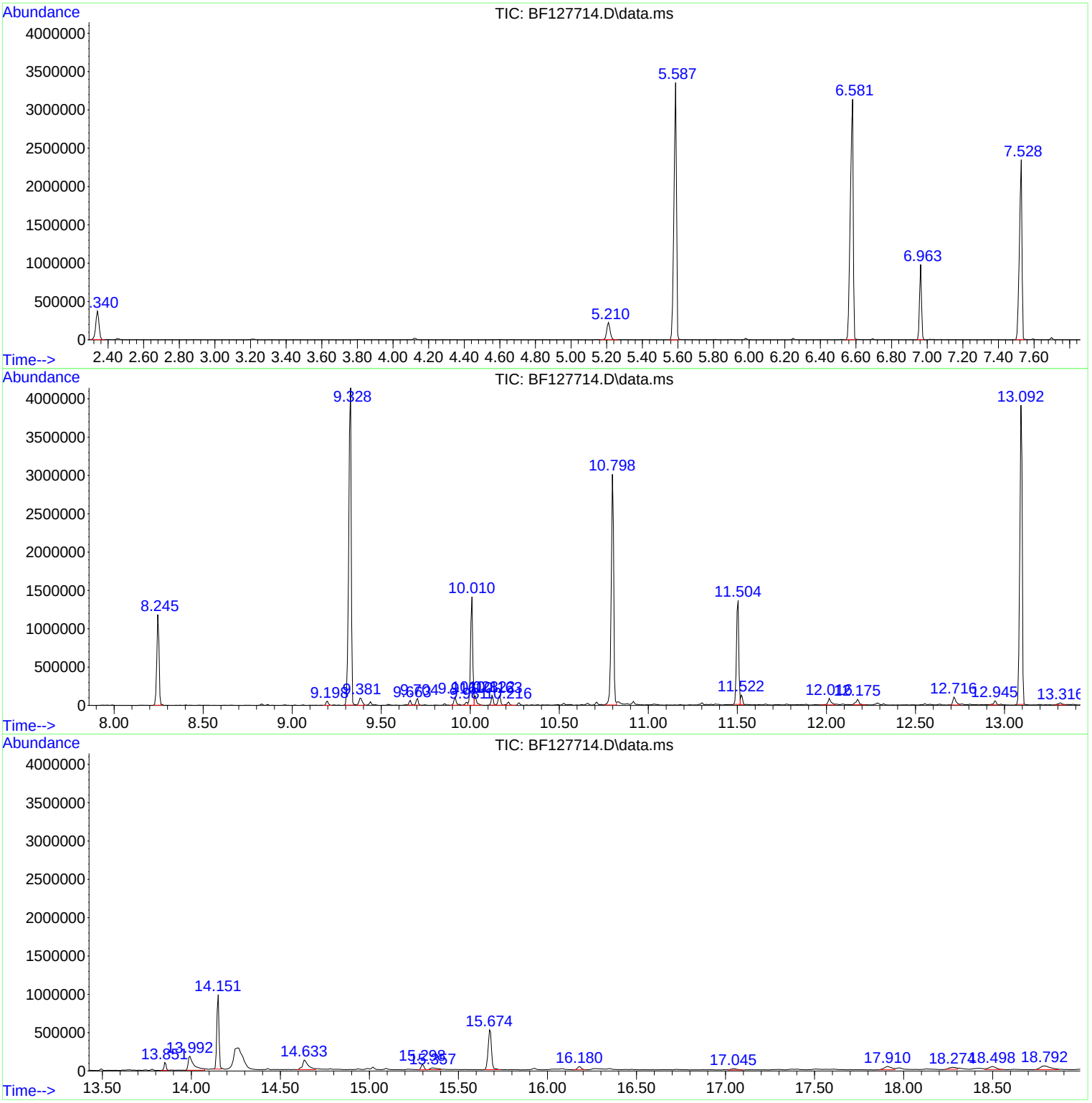
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BF127714.D
Acq On : 08 Apr 2022 15:29
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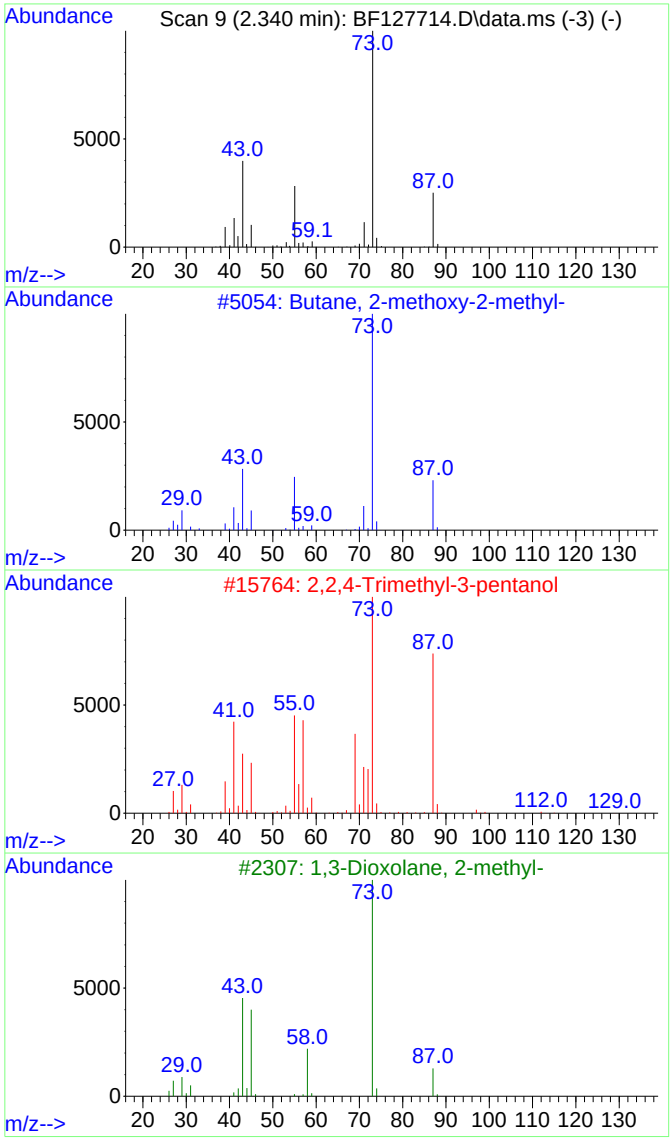
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

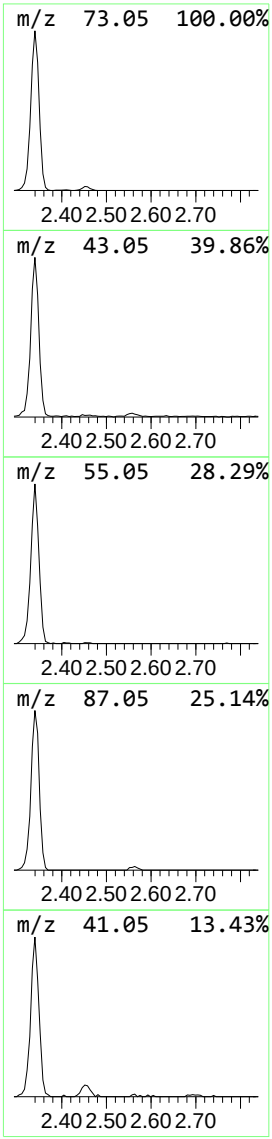
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.340	12.54 ng	479766	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	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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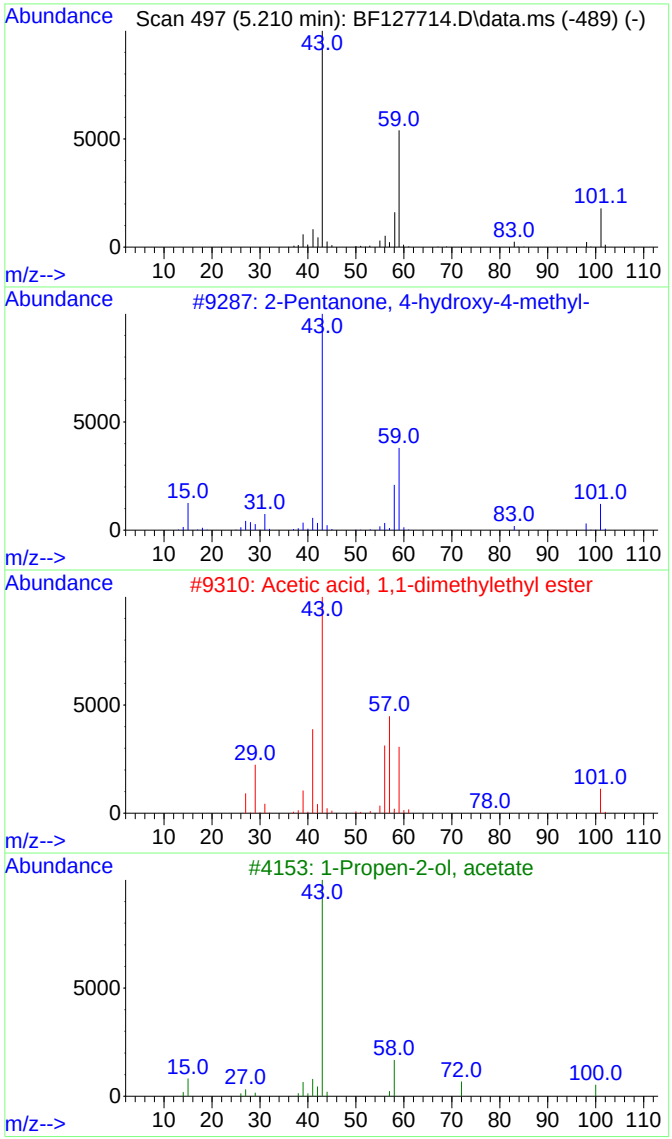
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

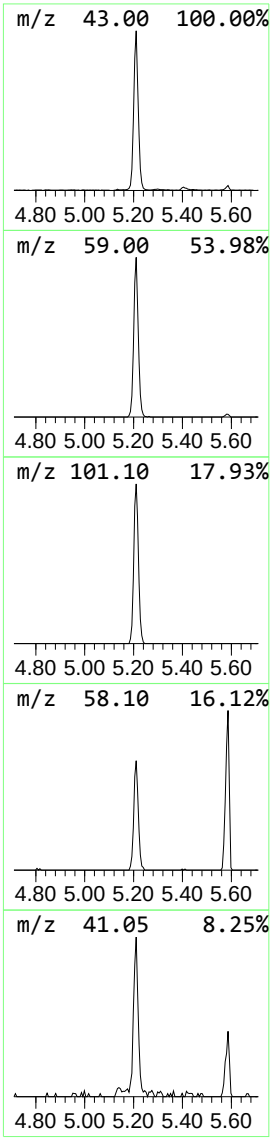
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.210	7.70 ng	294443	1,4-Dichlorobenzene-d4	6.963

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Sample : N2317-17
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

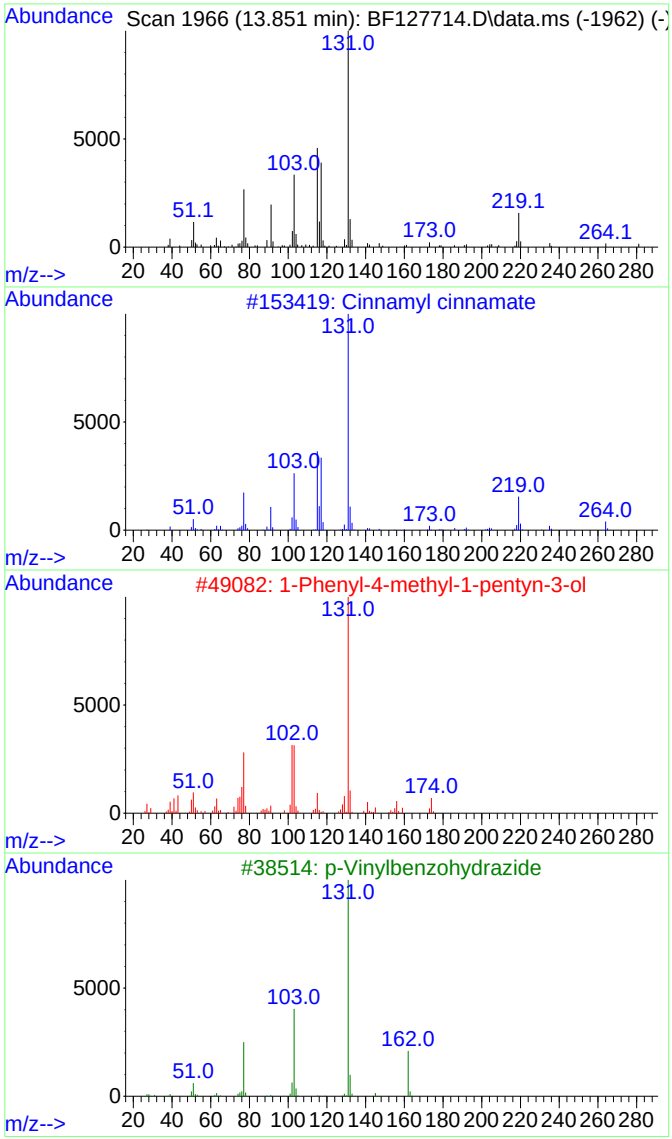
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

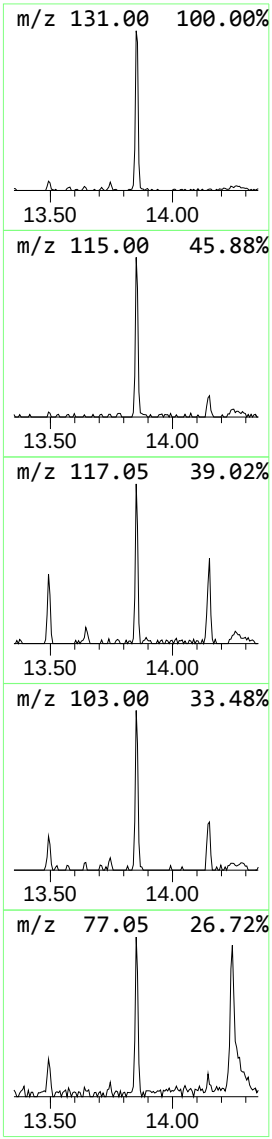
****

Peak Number 4 Cinnamyl cinnamate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	2.12 ng	88653	Chrysene-d12	14.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2	1-Phenyl-4-methyl-1-pentyn-3-ol	174	C12H14O	005923-02-4	47
3	p-Vinylbenzohydrazide	162	C9H10N2O	1000244-74-9	43
4	N-(4-Fluorophenyl)-3-phenyl-2-pr...	337	C17H11F4NO2	1000492-37-5	43
5	1-Penten-3-one, 4,4-dimethyl-1-p...	188	C13H16O	000538-44-3	43





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Operator : CG\JU
Sample : N2317-17
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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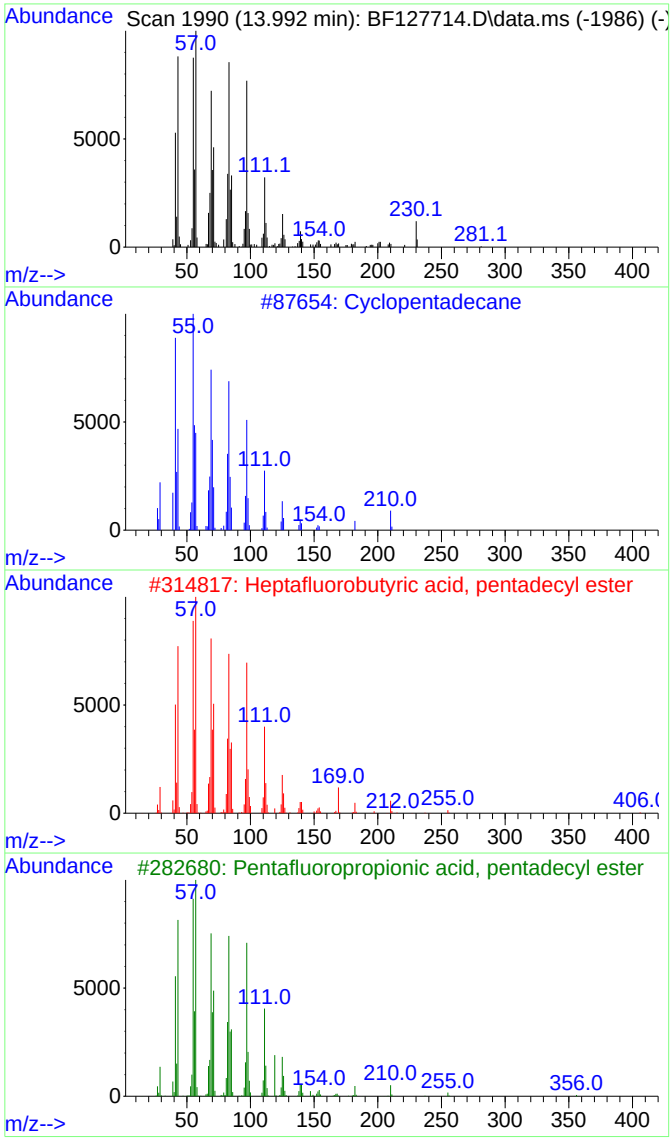
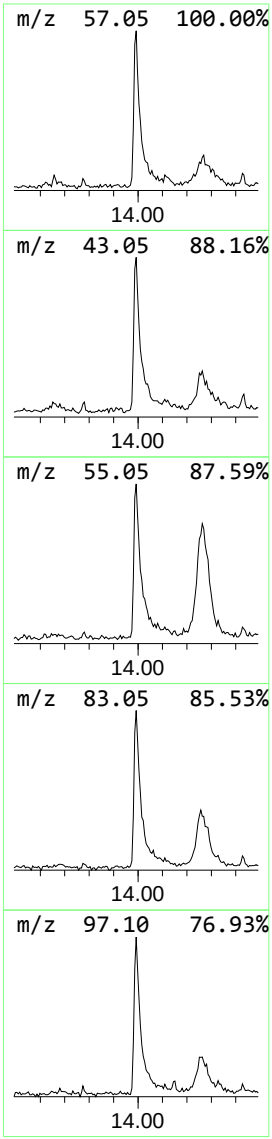
Peak Number 5 Cyclopentadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.992	9.65 ng	403161	Chrysene-d12	14.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	97
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

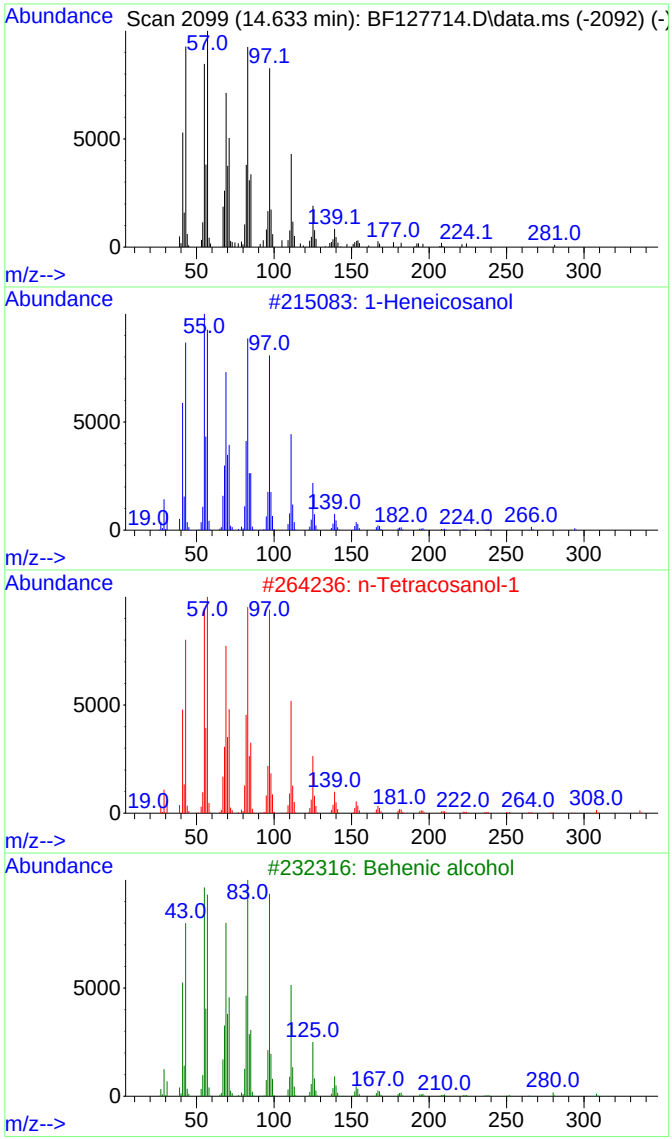
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

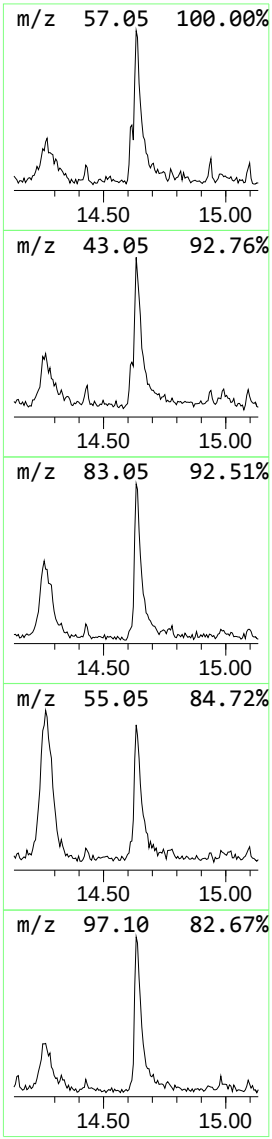
****

Peak Number 6 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.633	6.80 ng	284063	Chrysene-d12	14.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3	Behenic alcohol	326	C22H46O	000661-19-8	95
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	95
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94





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Sample : N2317-17
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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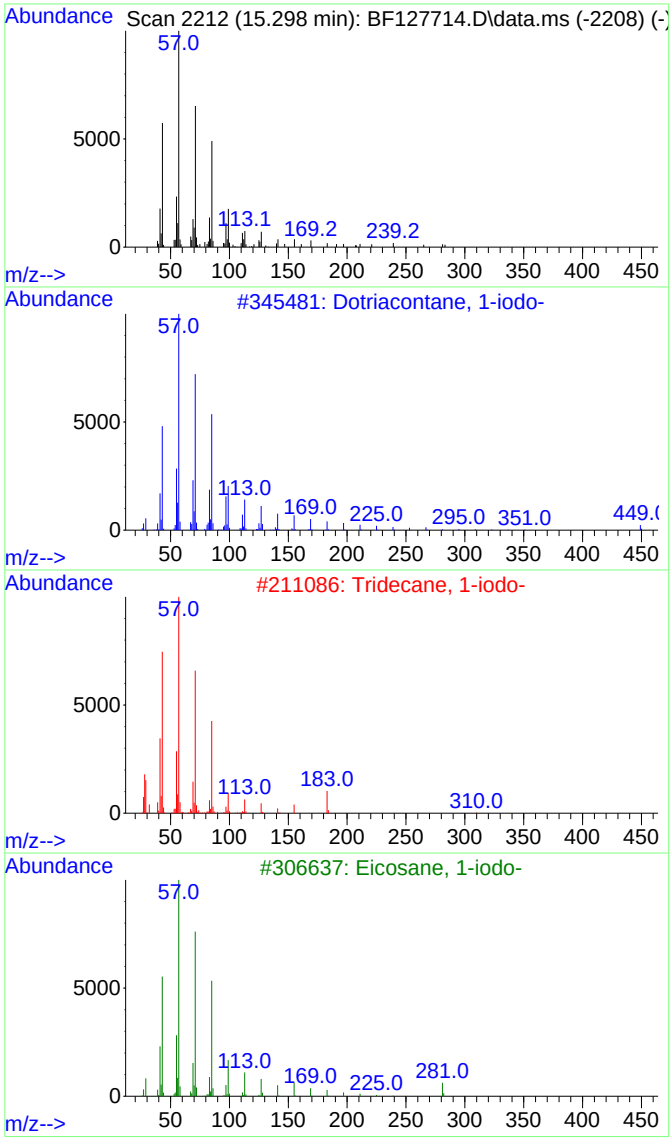
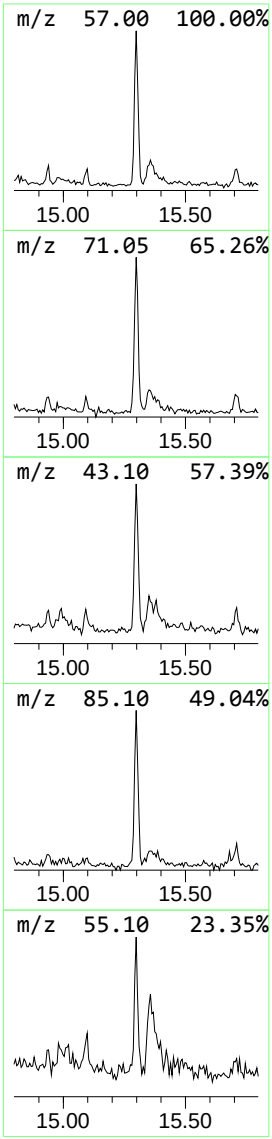
Peak Number 7 Dotriacontane, 1-iodo- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.298	2.27 ng	77685	Perylene-d12	15.674

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	90
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
3	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	86
4	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80





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Data File : BF127714.D
Acq On : 08 Apr 2022 15:29
Operator : CG\JU
Sample : N2317-17
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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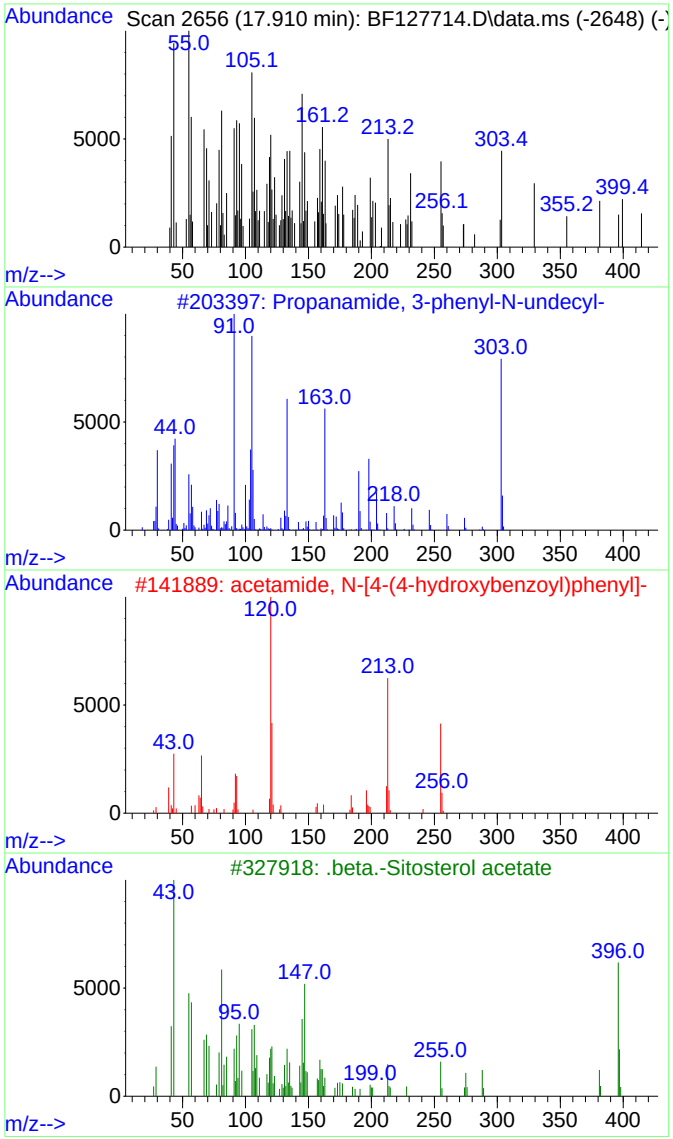
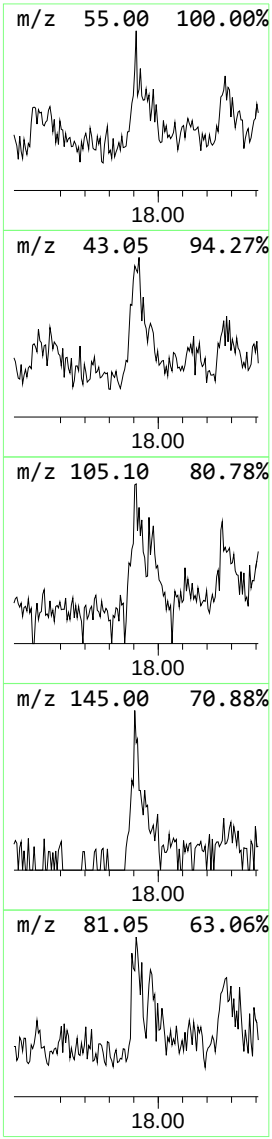
Peak Number 8 unknown17.910 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.910	3.66 ng	125404	Perylene-d12	15.674

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanamide, 3-phenyl-N-undecyl-	303	C20H33NO	1000407-15-8	18
2	acetamide, N-[4-(4-hydroxybenzoy...	255	C15H13NO3	1000396-71-2	14
3	.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	10
4	4-Acetyl-1-(3-ethoxypropyl)-3-hy...	303	C17H21NO4	1000387-64-4	9
5	.alpha.-D-Gglucopyranoside, meth...	418	C20H34O9	1000157-04-2	9





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Data File : BF127714.D
Acq On : 08 Apr 2022 15:29
Operator : CG\JU
Sample : N2317-17
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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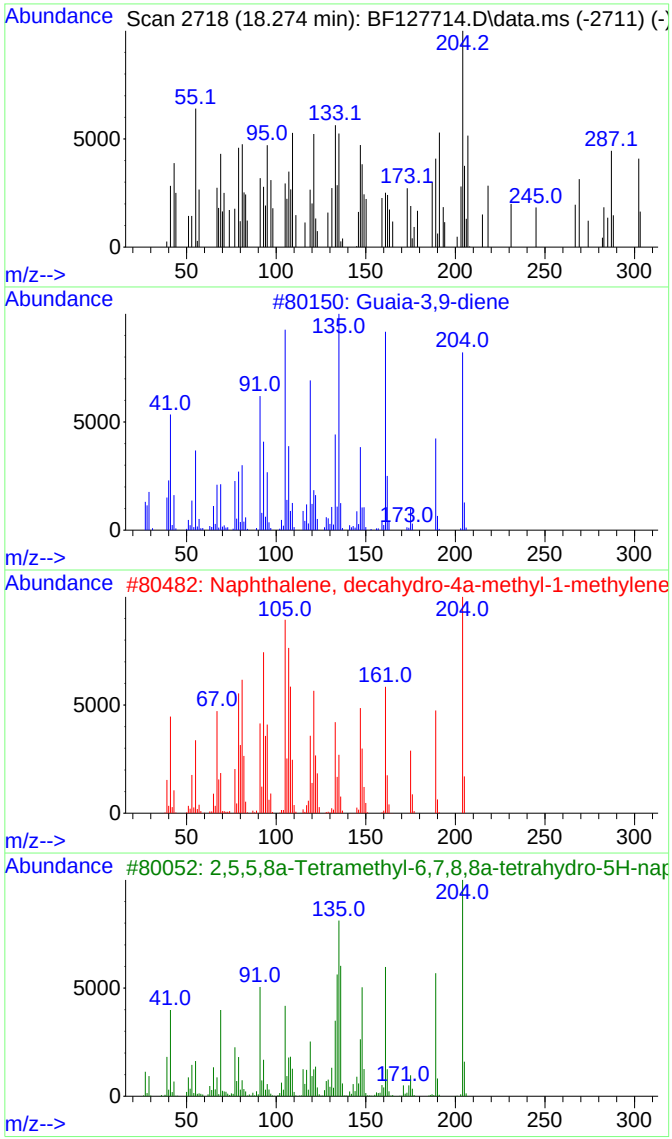
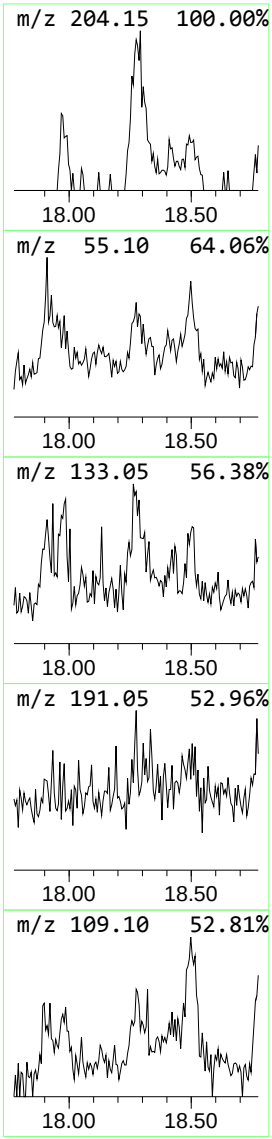
Peak Number 9 unknown18.274 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.274	2.20 ng	75521	Perylene-d12	15.674

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Guaia-3,9-diene	204	C15H24	000489-83-8	46
2	Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	43
3	2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H20O	124957-09-1	41
4	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	38
5	3-Chloro-5-fluoro-4-methoxybenzo...	204	C8H6ClFO3	886497-22-9	25





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Data File : BF127714.D
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Operator : CG\JU
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Misc :
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Instrument :
BNA_F
ClientSampleId :
TP1-A

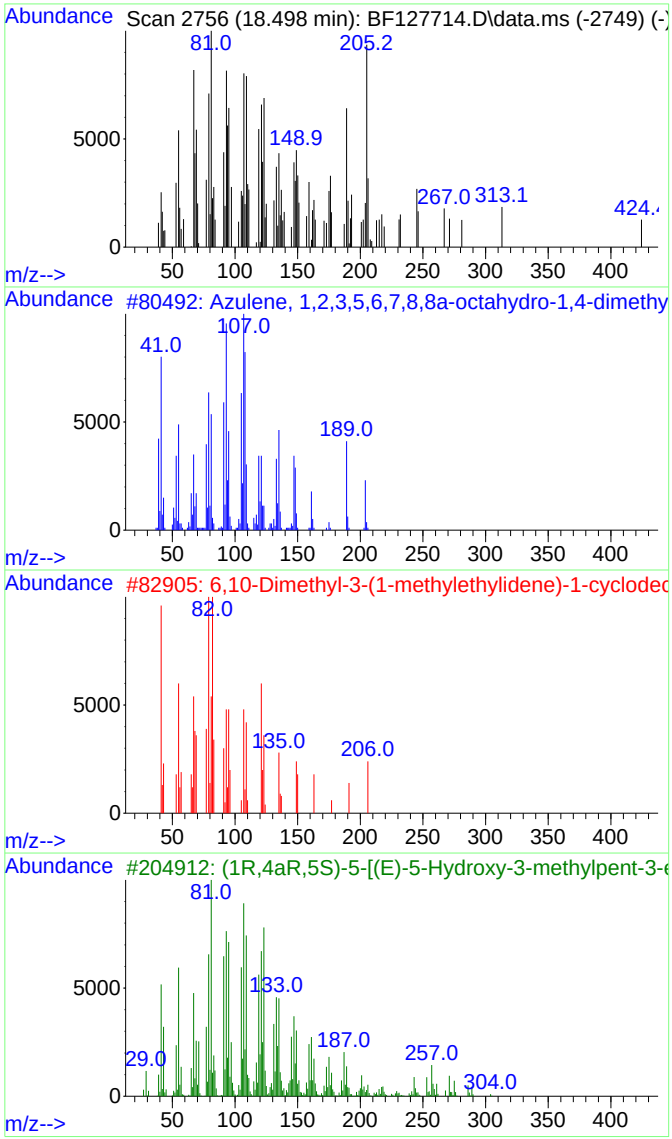
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

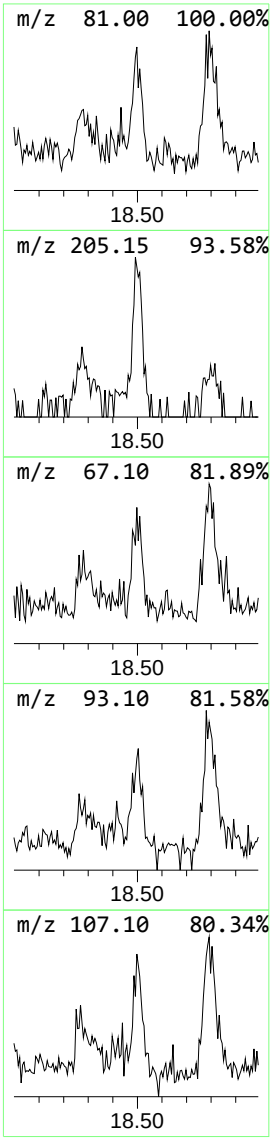
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Azulene, 1,2,3,5,6,7,8,8a-o... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.498	3.17 ng	108728	Perylene-d12	15.674

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Azulene, 1,2,3,5,6,7,8,8a-octahy...	204	C15H24	003691-11-0	60
2	6,10-Dimethyl-3-(1-methylethylid...	206	C15H26	069239-71-0	46
3	(1R,4aR,5S)-5-[(E)-5-Hydroxy-3-m...	304	C20H32O2	1214984-94-7	46
4	Guaia-9,11-diene	204	C15H24	1000374-19-8	42
5	4a,8-Dimethyl-2-(prop-1-en-2-yl)...	204	C15H24	103827-22-1	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040822\
Data File : BF127714.D
Acq On : 08 Apr 2022 15:29
Operator : CG\JU
Sample : N2317-17
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-A

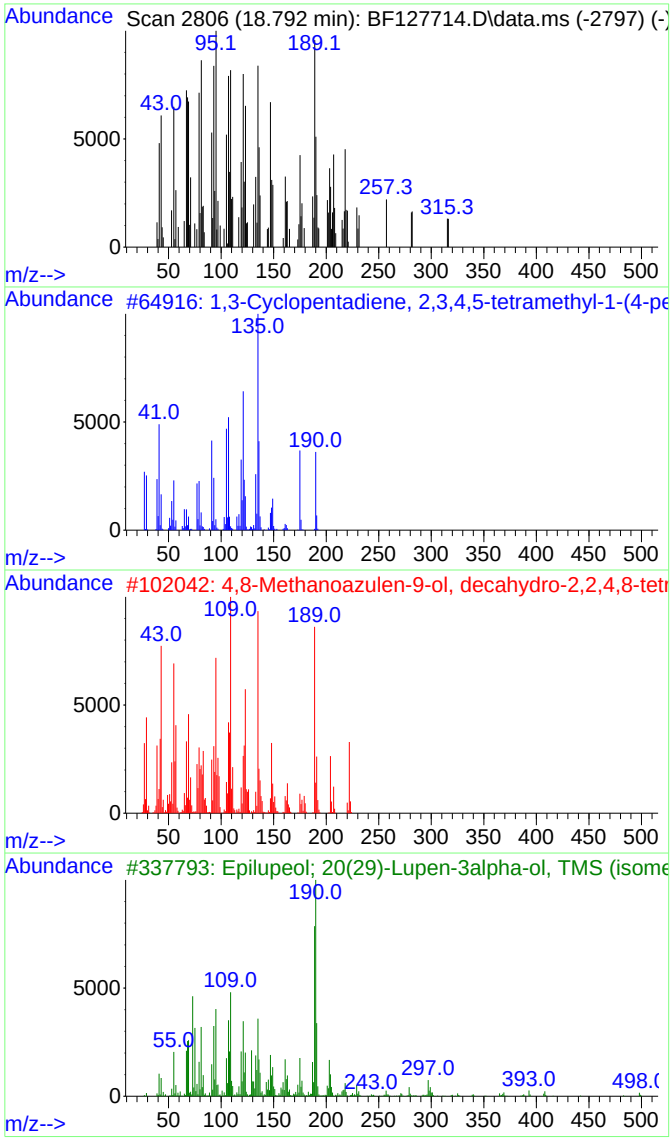
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

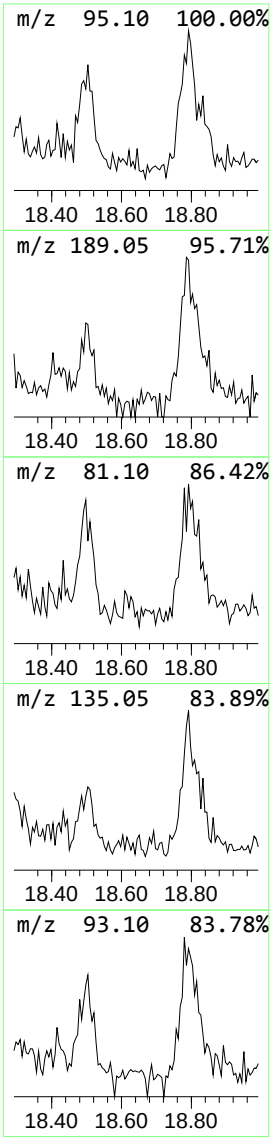
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 1,3-Cyclopentadiene, 2,3,4,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.792	5.53 ng	189280	Perylene-d12	15.674

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentadiene, 2,3,4,5-tet...	190	C14H22	1000161-28-7	51
2	4,8-Methanoazulen-9-ol, decahydr...	222	C15H26O	004586-22-5	46
3	Epilupeol; 20(29)-Lupen-3alpha-o...	498	C33H58OSi	1000513-01-6	46
4	(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	45
5	1,5-Cyclodecadiene, 1,5-dimethyl...	204	C15H24	075023-40-4	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040822\
Data File : BF127714.D
Acq On : 08 Apr 2022 15:29
Operator : CG\JU
Sample : N2317-17
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
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...	2.340	12.5	ng	479766	1	6.963	765049	20.0
2-Pentanone, 4-...	5.210	7.7	ng	294443	1	6.963	765049	20.0
Cinnamyl cinnamate	13.851	2.1	ng	88653	5	14.151	835626	20.0
Cyclopentadecane	13.992	9.7	ng	403161	5	14.151	835626	20.0
1-Heneicosanol	14.633	6.8	ng	284063	5	14.151	835626	20.0
Dotriacontane, ...	15.298	2.3	ng	77685	6	15.674	685132	20.0
unknown17.910	17.910	3.7	ng	125404	6	15.674	685132	20.0
unknown18.274	18.274	2.2	ng	75521	6	15.674	685132	20.0
Azulene, 1,2,3,...	18.498	3.2	ng	108728	6	15.674	685132	20.0
1,3-Cyclopentad...	18.792	5.5	ng	189280	6	15.674	685132	20.0