LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080322\
Data File : BF129551.D
Acq On : 03 Aug 2022 21:04
Operator : CG\JU
Sample : N3930-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RVE-104

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-BF072522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129551.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.093	474	477	484	rVB	35115	42480	1.99%	0.220%
2	5.499	542	546	560	rBV	2364937	2133163	99.72%	11.057%
3	6.510	714	718	732	rBV	2444027	2039965	95.37%	10.574%
4	6.869	775	779	782	rBV	904895	727303	34.00%	3.770%
5	7.428	870	874	878	rBV	1364652	1307876	61.14%	6.779%
6	8.151	993	997	1000	rBV	1065775	863115	40.35%	4.474%
7	9.222	1175	1179	1182	rBV	2585647	2139107	100.00%	11.087%
8	9.904	1291	1295	1299	rBV	888459	771423	36.06%	3.998%
9	10.698	1426	1430	1439	rBV	1225096	1012442	47.33%	5.248%
10	11.398	1545	1549	1552	rBV	739245	659491	30.83%	3.418%
11	11.910	1629	1636	1641	rBV3	35849	60736	2.84%	0.315%
12	12.610	1752	1755	1759	rVB	79267	65613	3.07%	0.340%
13	12.839	1789	1794	1797	rBV	82054	81496	3.81%	0.422%
14	12.980	1814	1818	1821	rBV	2163336	1784799	83.44%	9.251%
15	13.198	1851	1855	1859	rVB	35055	35330	1.65%	0.183%
16	13.539	1909	1913	1916	rBV2	38397	46944	2.19%	0.243%
17	13.657	1930	1933	1935	rBV2	39151	34231	1.60%	0.177%
18	13.874	1966	1970	1982	rBV3	230386	494147	23.10%	2.561%
19	14.039	1994	1998	2001	rBV	936041	839250	39.23%	4.350%
20	14.063	2001	2002	2009	rVB	50247	47717	2.23%	0.247%
21	14.133	2011	2014	2018	rVB2	23324	28998	1.36%	0.150%
22	14.186	2020	2023	2025	rBV2	39406	38619	1.81%	0.200%
23	14.457	2066	2069	2072	rBV2	67139	60840	2.84%	0.315%
24	14.486	2072	2074	2076	rBV	120743	100204	4.68%	0.519%
25	14.516	2076	2079	2083	rVV5	45529	73514	3.44%	0.381%
26	14.798	2124	2127	2130	rVB2	34354	35741	1.67%	0.185%
27	14.874	2137	2140	2144	rVB	49668	50302	2.35%	0.261%
28	14.945	2149	2152	2156	rVB2	73337	74869	3.50%	0.388%
29	15.086	2173	2176	2179	rBV	47480	61942	2.90%	0.321%
30	15.133	2181	2184	2189	rVB	147287	172025	8.04%	0.892%
31	15.398	2226	2229	2235	rVB	38230	56907	2.66%	0.295%
32	15.457	2237	2239	2244	rVB	41165	50806	2.38%	0.263%
33	15.527	2246	2251	2255	rVV	698196	849606	39.72%	4.404%
34	15.727	2282	2285	2290	rVB	71291	86815	4.06%	0.450%
35	15.957	2320	2324	2330	rVB	217029	320399	14.98%	1.661%
36	16.774	2458	2463	2469	rVB2	101398	182909	8.55%	0.948%

LSC Area Percent Report

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Acq On : 03 Aug 2022 21:04
Operator : CG\JU
Sample : N3930-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-104

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-BF072522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.174	2524	2531	2543	rBV2	468322	1148913	53.71%	5.955%
38	17.515	2584	2589	2596	rVB9	74048	173110	8.09%	0.897%
39	17.627	2602	2608	2623	rVB9	80814	267070	12.49%	1.384%
40	18.639	2774	2780	2793	rVB4	88605	272804	12.75%	1.414%

Sum of corrected areas: 19293021

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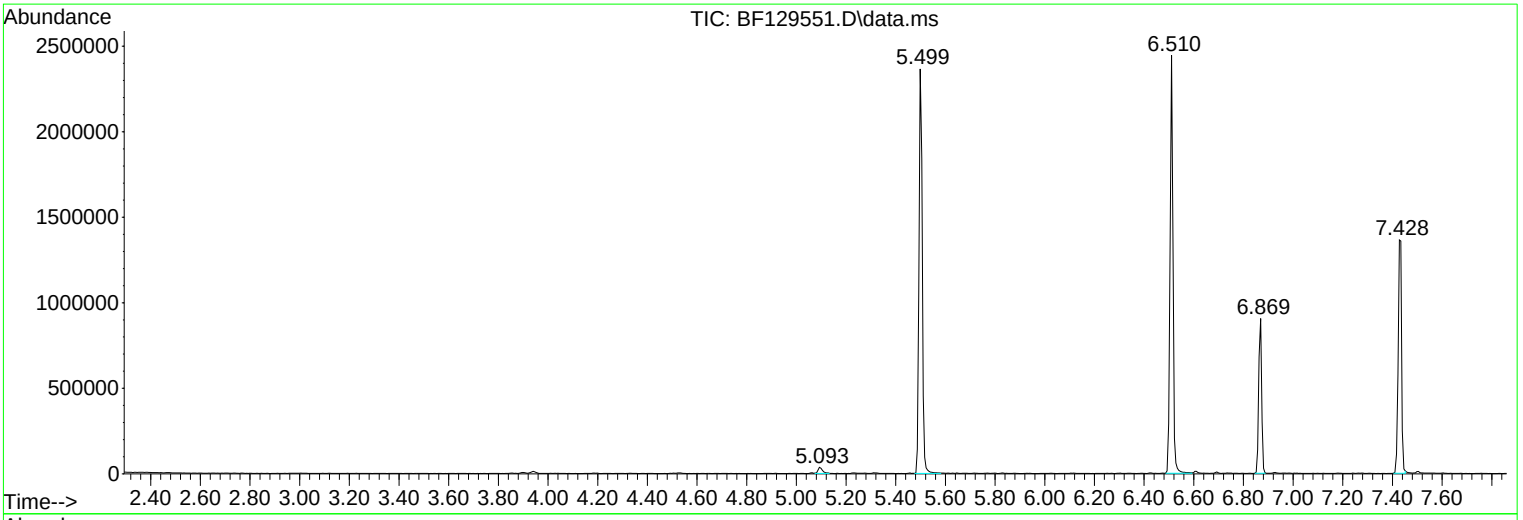
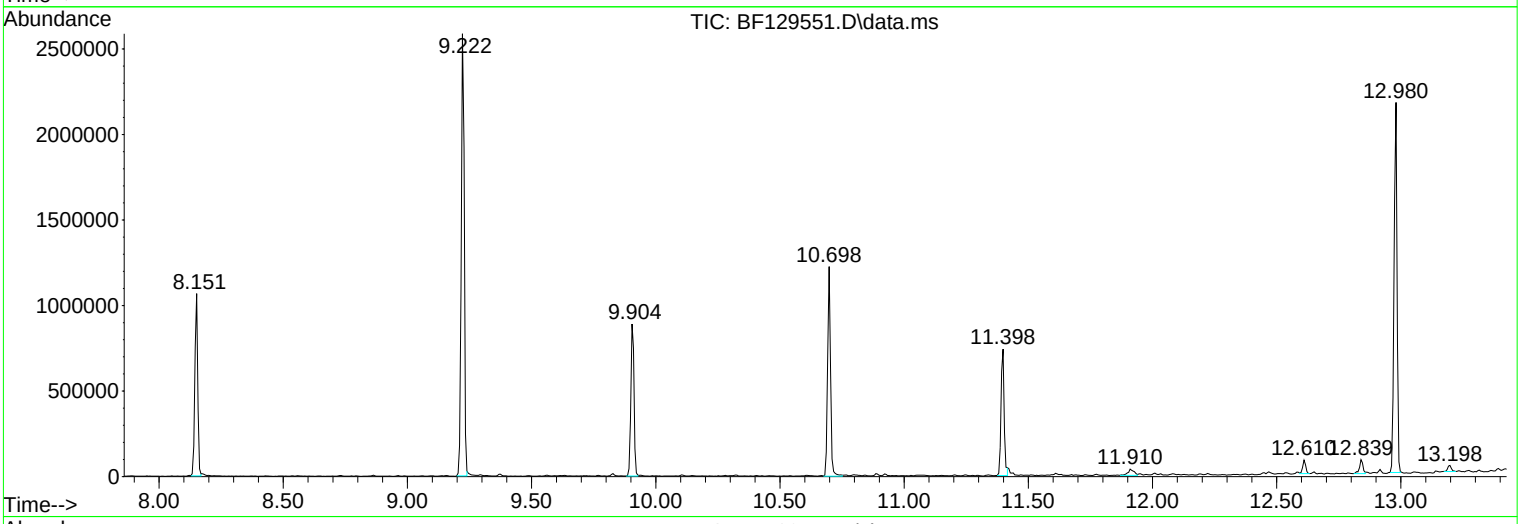
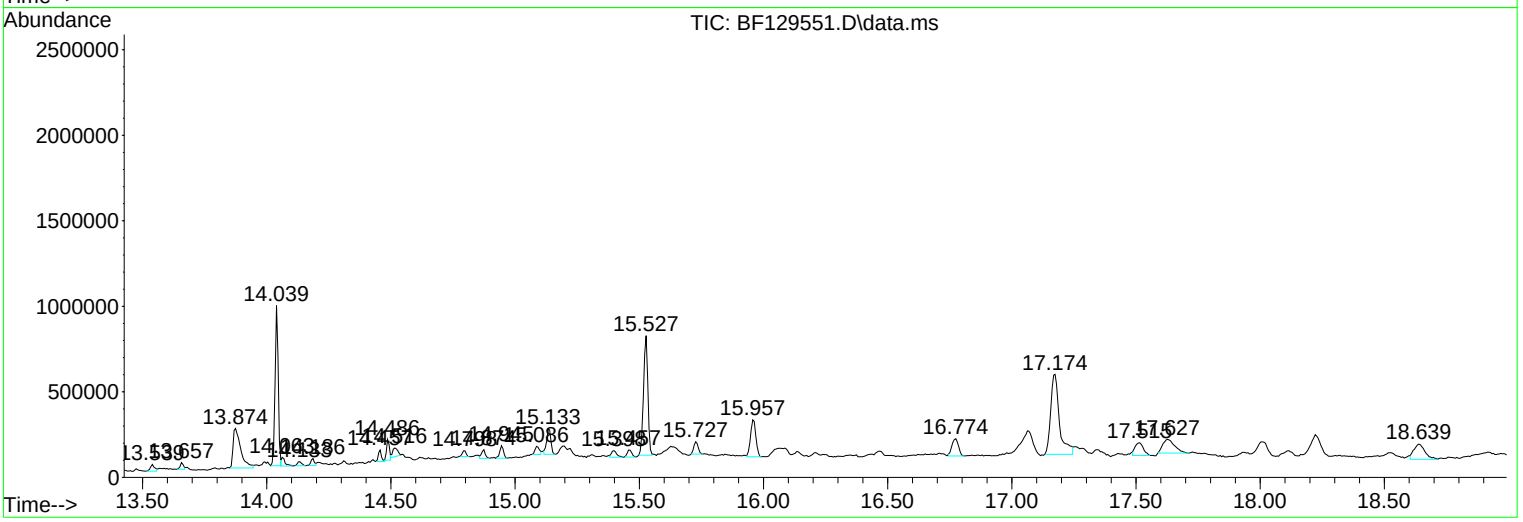
Instrument :
BNA_F
ClientSampleId :
RVE-104

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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\BF080322\
Data File : BF129551.D
Acq On : 03 Aug 2022 21:04
Operator : CG\JU
Sample : N3930-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-104

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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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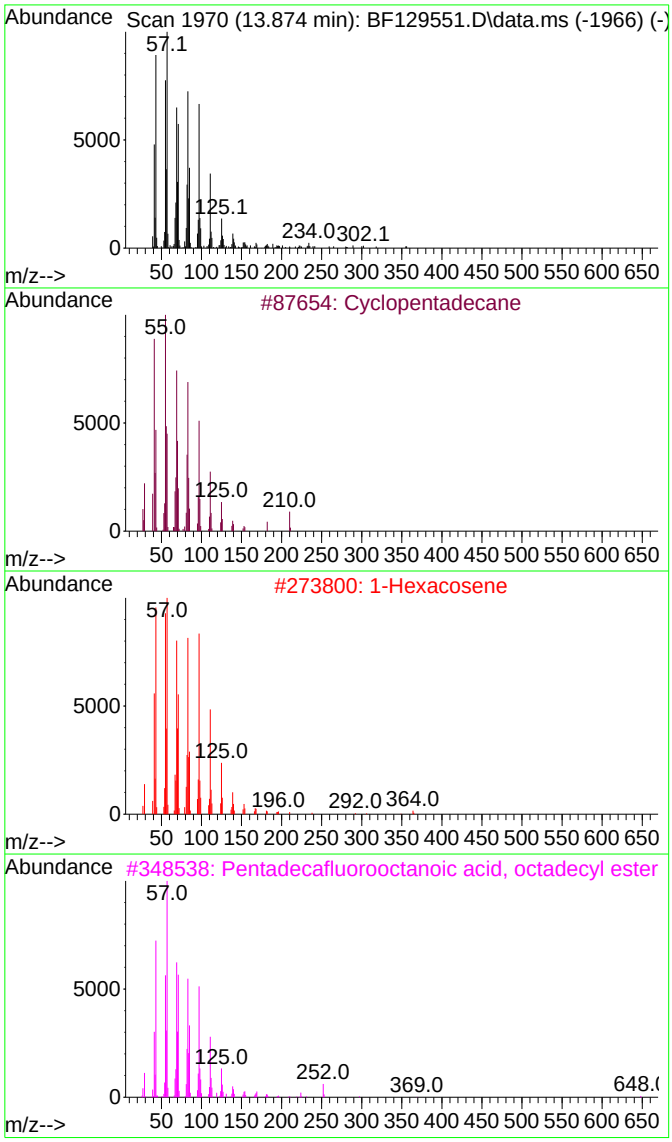
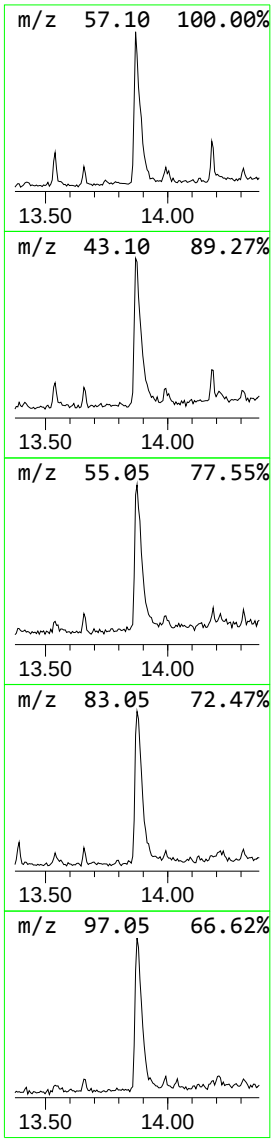
Peak Number 1 Cyclopentadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	11.78 ng	494147	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	95
2	1-Hexacosene	364	C26H52	018835-33-1	94
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91





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Operator : CG\JU
Sample : N3930-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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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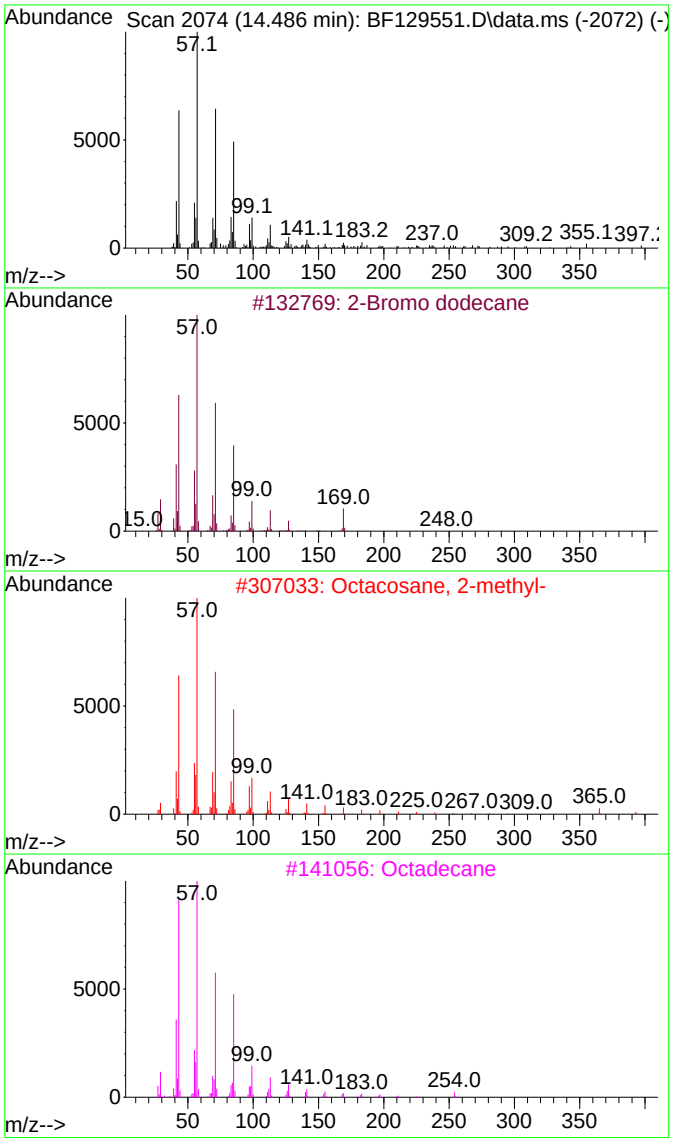
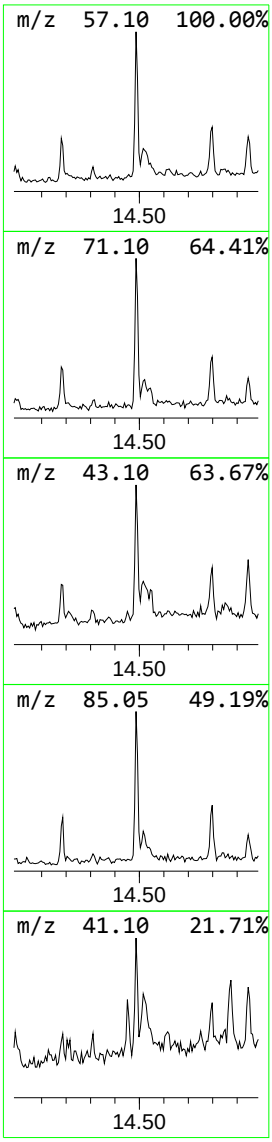
Peak Number 2 2-Bromo dodecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.486	2.39 ng	100204	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	93
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
3	Octadecane	254	C18H38	000593-45-3	87
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5	Docosane	310	C22H46	000629-97-0	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080322\
Data File : BF129551.D
Acq On : 03 Aug 2022 21:04
Operator : CG\JU
Sample : N3930-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-104

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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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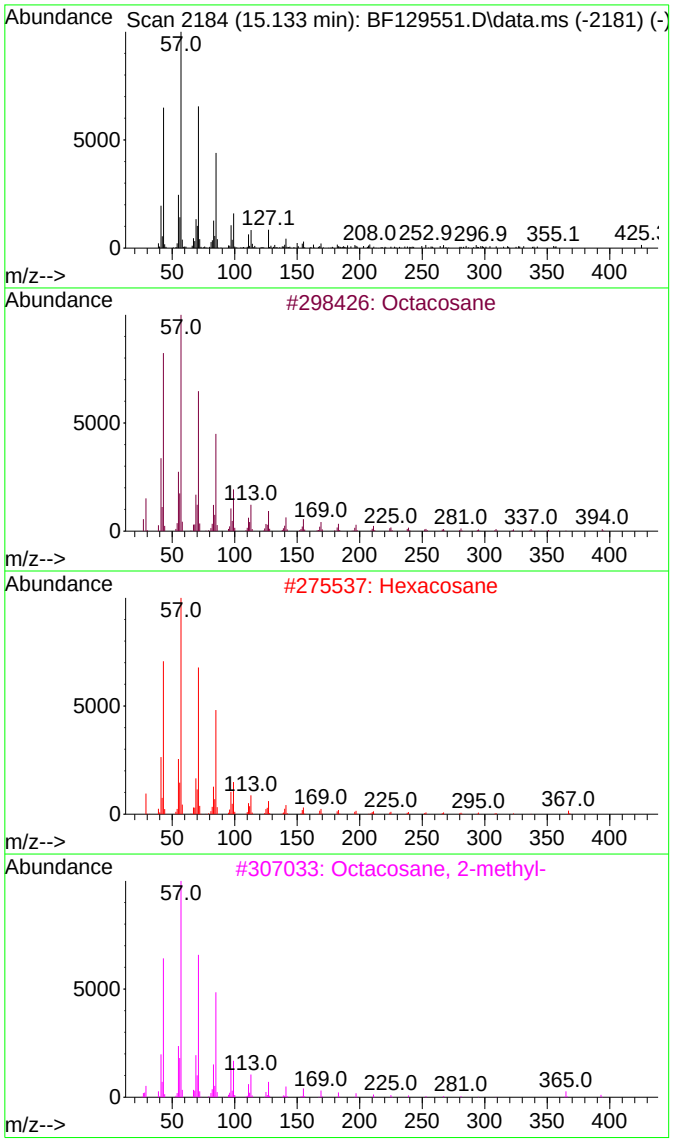
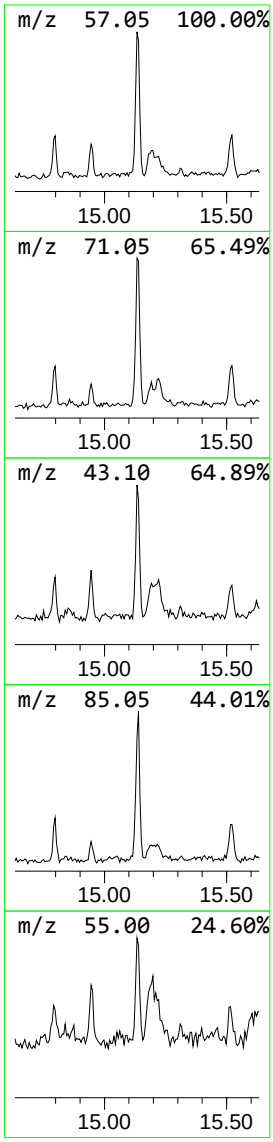
Peak Number 3 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.133	4.05 ng	172025	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5	Heneicosane	296	C21H44	000629-94-7	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080322\
Data File : BF129551.D
Acq On : 03 Aug 2022 21:04
Operator : CG\JU
Sample : N3930-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-104

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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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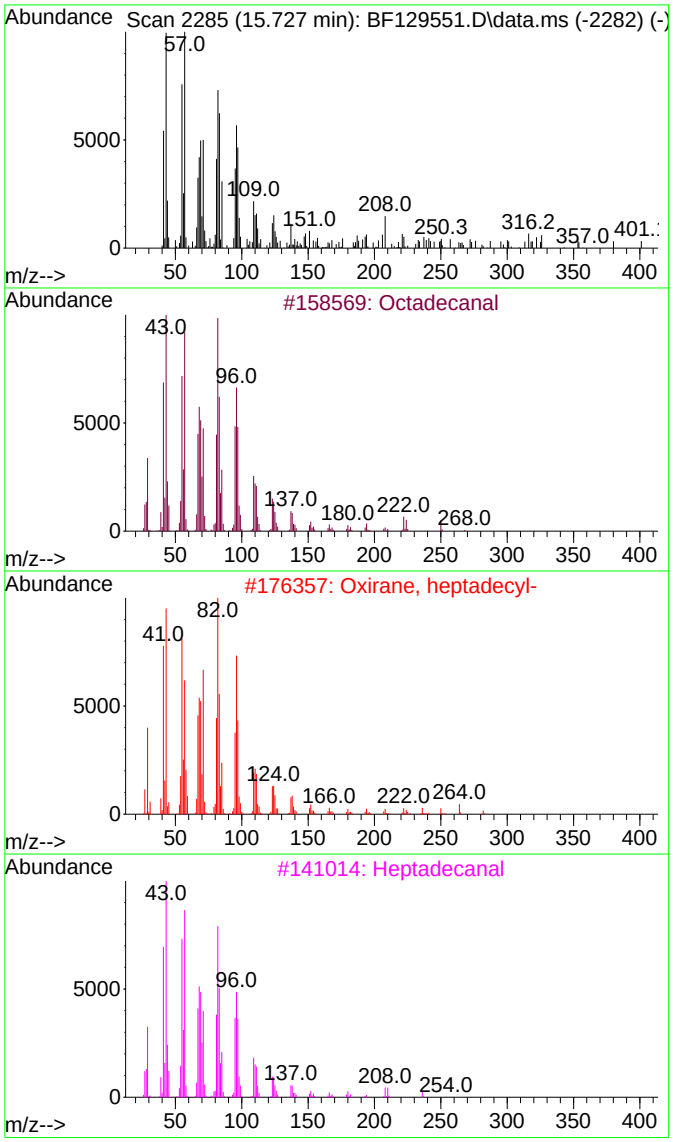
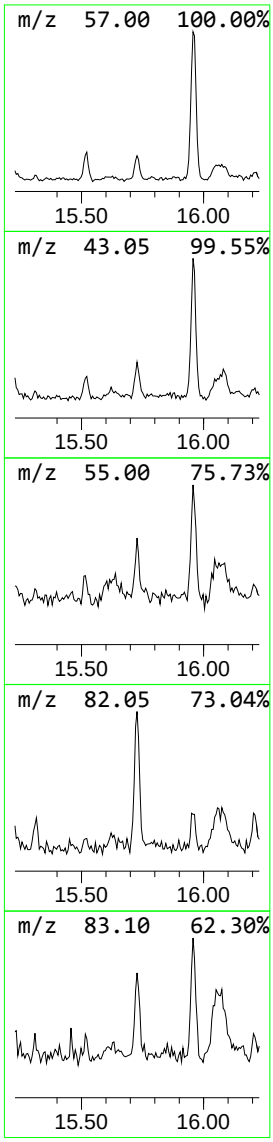
Peak Number 4 Octadecanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.727	2.04 ng	86815	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	90
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	89
3	Heptadecanal	254	C17H34O	1000376-70-0	87
4	Eicosanal-	296	C20H40O	002400-66-0	87
5	Z-11,13-Dimethyl-11-tetradecen-1...	282	C18H34O2	1000131-36-6	84





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080322\
Data File : BF129551.D
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Operator : CG\JU
Sample : N3930-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-104

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

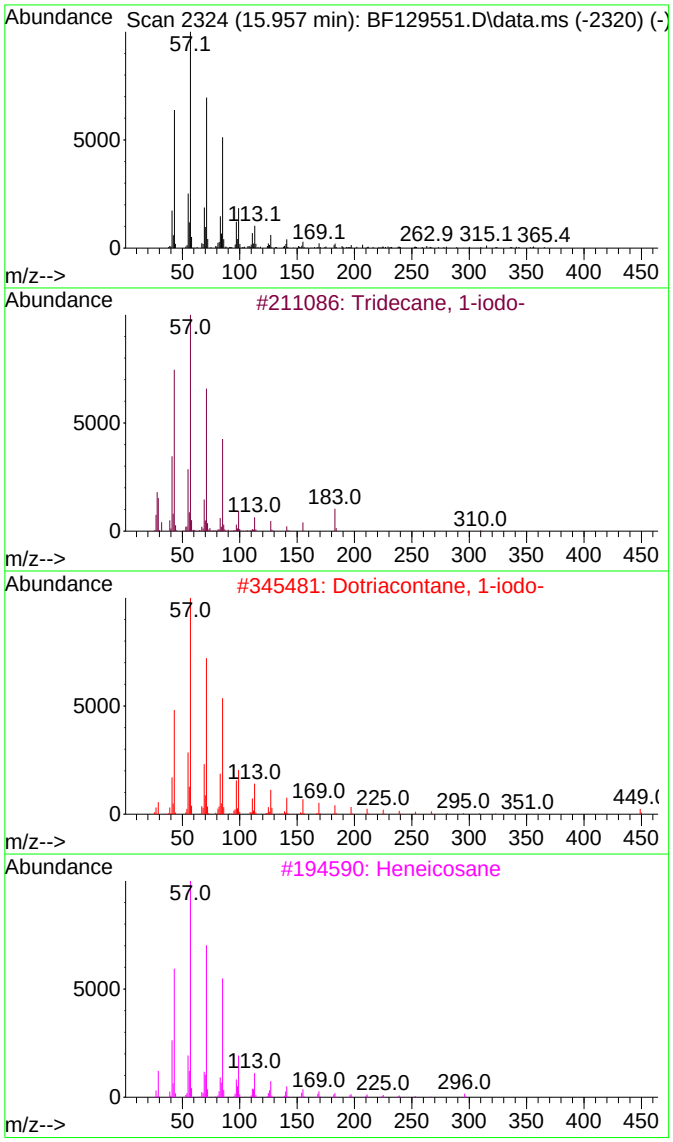
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

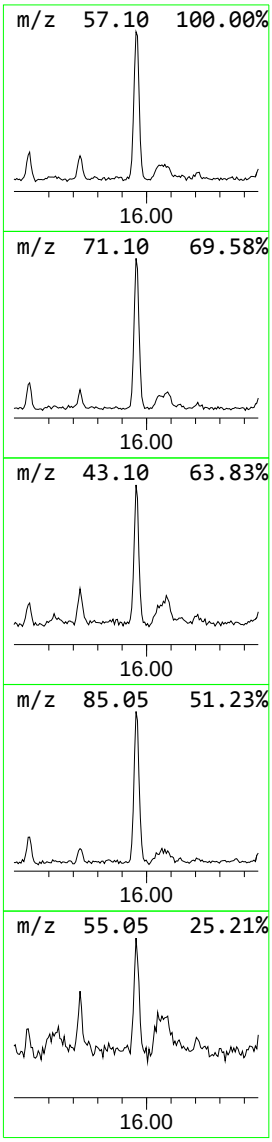
****

Peak Number 5 Tridecane, 1-iodo- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.957	7.54 ng	320399	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	93
2	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5	Heptadecane	240	C17H36	000629-78-7	90





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Operator : CG\JU
Sample : N3930-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-104

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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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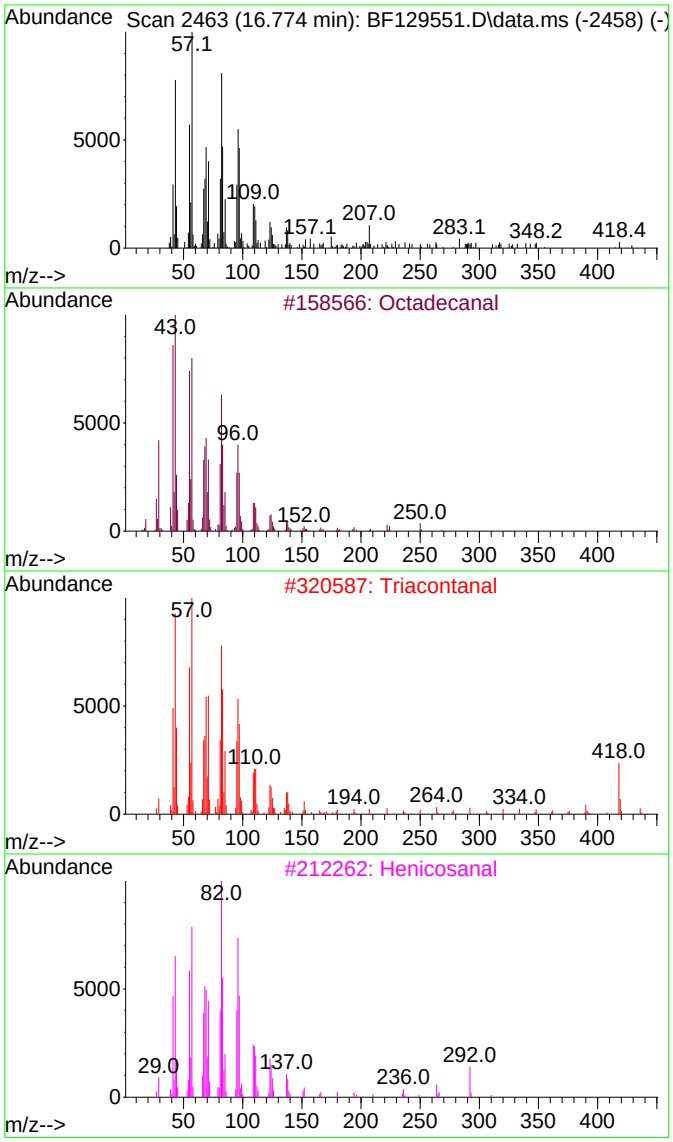
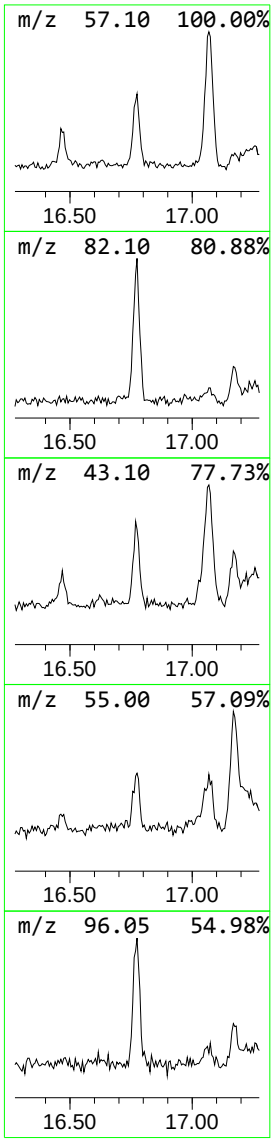
Peak Number 6 Triacontanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.774	4.31 ng	182909	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	90
2	Triacontanal	436	C30H60O	022725-63-9	86
3	Henicosanal	310	C21H42O	051227-32-8	81
4	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	74
5	1,19-Eicosadiene	278	C20H38	014811-95-1	72





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Sample : N3930-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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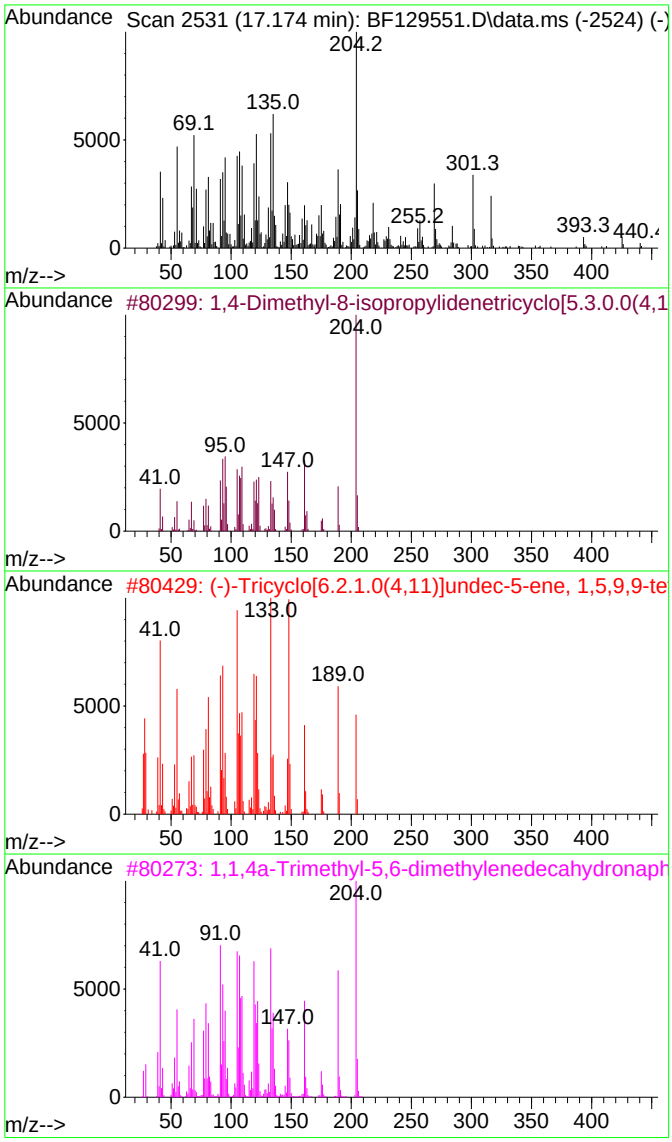
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

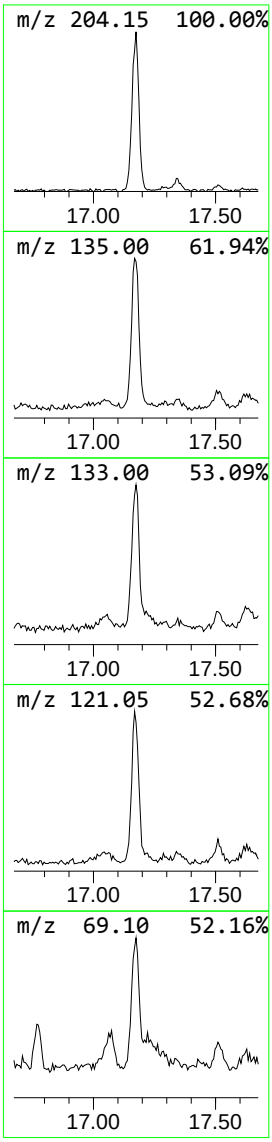
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1,4-Dimethyl-8-isopropylide... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.174	27.05 ng	1148910	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1010140-07-7	76
2	(-)-Tricyclo[6.2.1.0(4,11)]undec...	204	C15H24	1000154-06-7	72
3	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	59
4	(S,E)-8,12,15,15-Tetramethyl-4-m...	272	C20H32	386223-19-4	55
5	Farnesyl bromide	284	C15H25Br	006874-67-5	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080322\
Data File : BF129551.D
Acq On : 03 Aug 2022 21:04
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Sample : N3930-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-104

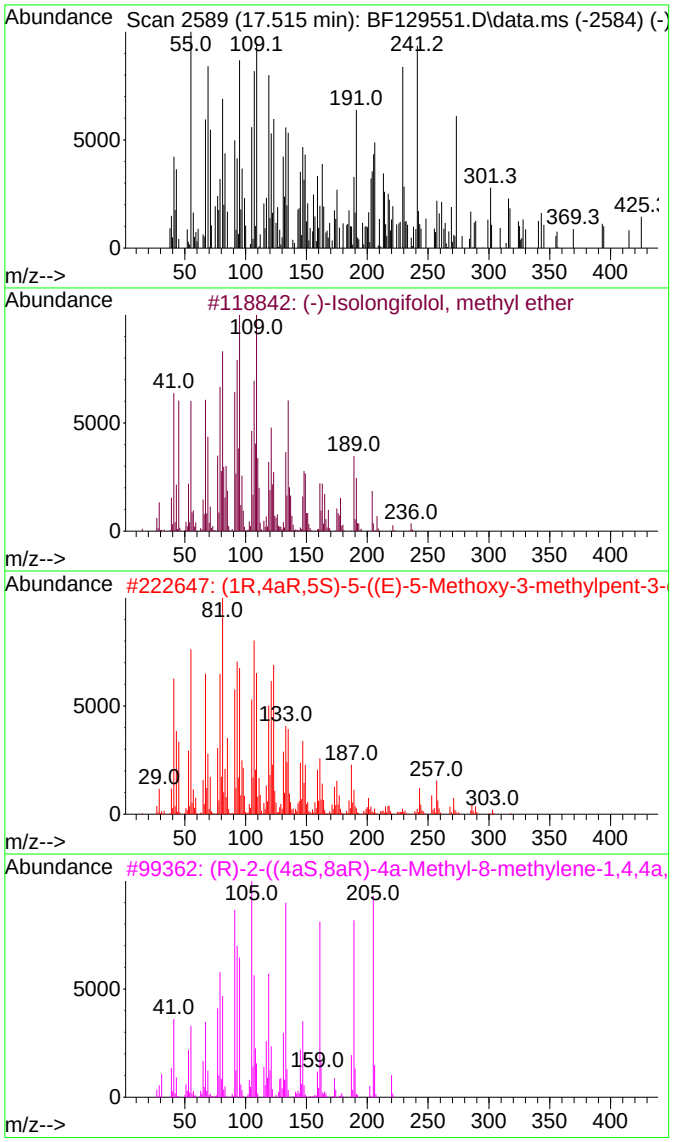
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

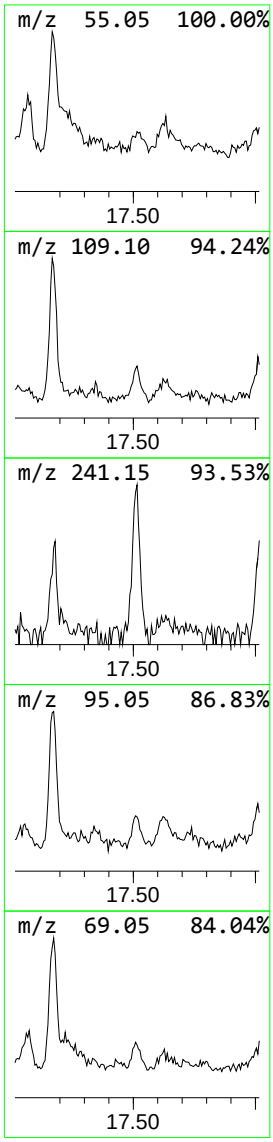
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 (-)-Isolongifolol, methyl e... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.515	4.08 ng	173110	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(-)-Isolongifolol, methyl ether	236	C16H28O	1000333-80-8	56
2	(1R,4aR,5S)-5-((E)-5-Methoxy-3-m...	318	C21H34O2	1000495-78-7	38
3	(R)-2-((4aS,8aR)-4a-Methyl-8-met...	220	C15H24O	028102-68-3	30
4	(1aR,4aS,8aS)-4a,8,8-Trimethyl-1...	218	C15H22O	000470-41-7	25
5	4-(6,6-Dimethyl-2-methylenecyclo...	206	C14H22O	1000195-14-3	25





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Data File : BF129551.D
Acq On : 03 Aug 2022 21:04
Operator : CG\JU
Sample : N3930-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-104

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

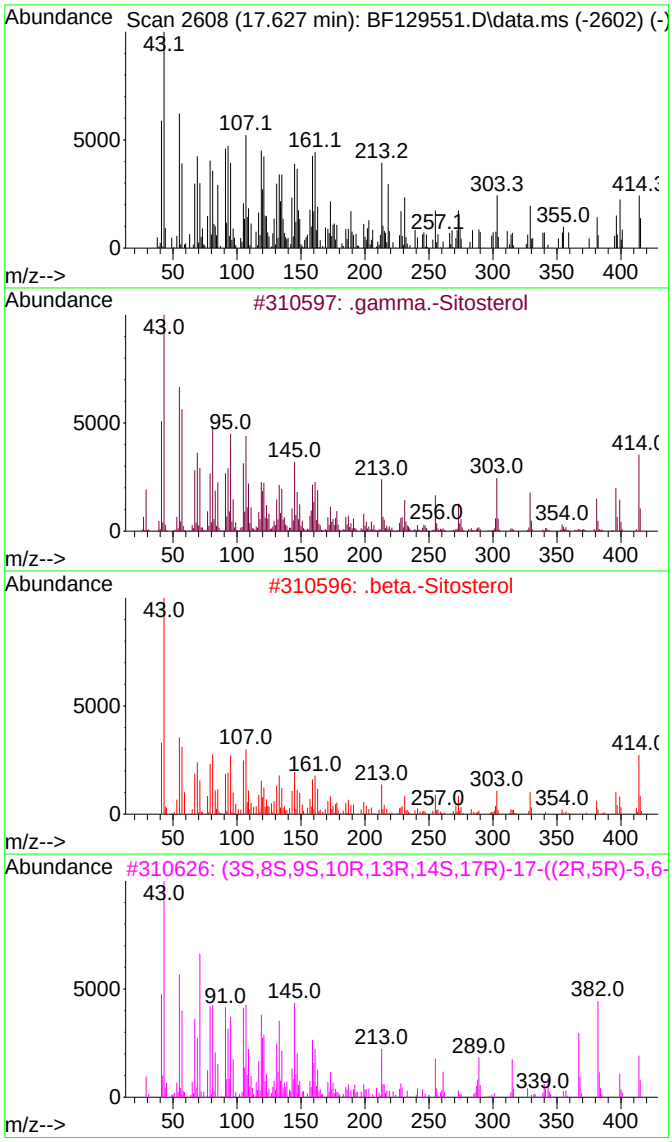
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

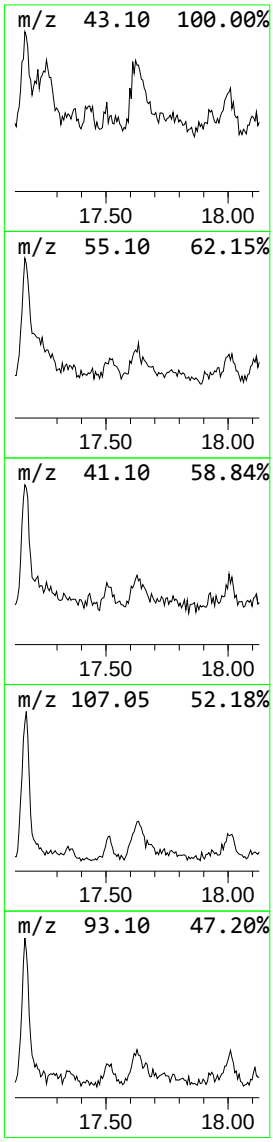
****

Peak Number 9 .gamma.-Sitosterol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.627	6.29 ng	267070	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	94
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	89
3	(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	32
4	Ergost-5-en-3-ol, (3.beta.)-	400	C28H48O	004651-51-8	17
5	Cholest-7-en-3-ol, 4,4-dimethyl-...	414	C29H50O	006384-28-7	15





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080322\
Data File : BF129551.D
Acq On : 03 Aug 2022 21:04
Operator : CG\JU
Sample : N3930-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-104

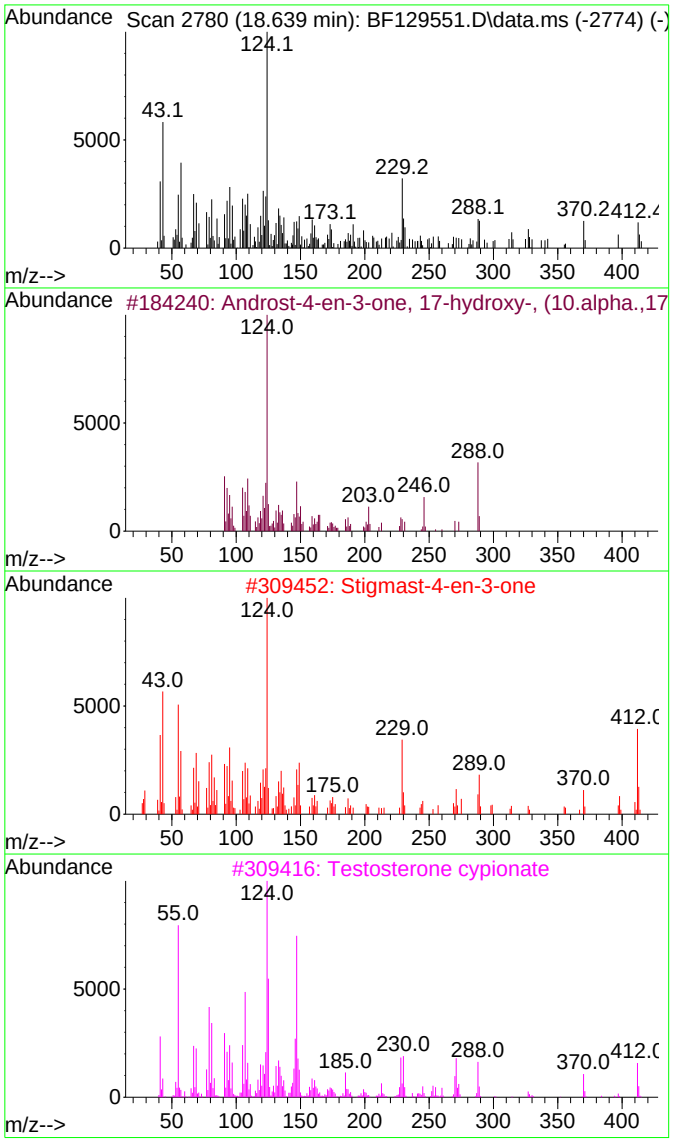
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

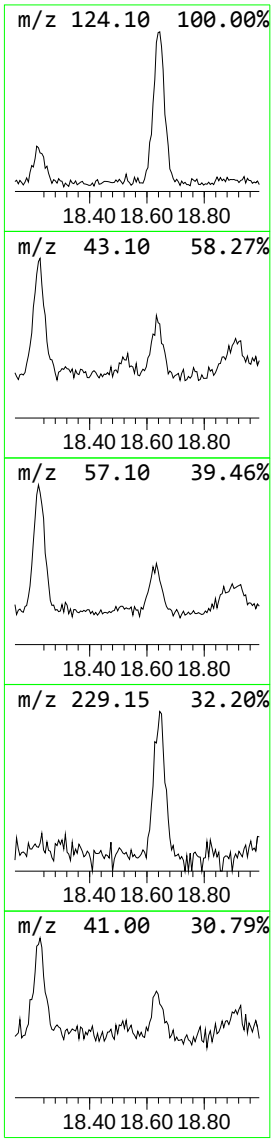
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Androst-4-en-3-one, 17-hydr... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.639	6.42 ng	272804	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Androst-4-en-3-one, 17-hydroxy-,...	288	C19H28O2	000604-39-7	83
2	Stigmast-4-en-3-one	412	C29H48O	001058-61-3	80
3	Testosterone cypionate	412	C27H40O3	000058-20-8	62
4	17beta-Acetoxy-10-isoandrost-4-e...	330	C21H30O3	002681-55-2	53
5	.gamma.-Sitostenone	412	C29H48O	084924-96-9	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080322\
Data File : BF129551.D
Acq On : 03 Aug 2022 21:04
Operator : CG\JU
Sample : N3930-12
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-104

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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
Cyclopentadecane	13.874	11.8	ng	494147	5	14.039	839250	20.0
2-Bromo dodecane	14.486	2.4	ng	100204	5	14.039	839250	20.0
Octacosane	15.133	4.0	ng	172025	6	15.527	849606	20.0
Octadecanal	15.727	2.0	ng	86815	6	15.527	849606	20.0
Tridecane, 1-iodo-	15.957	7.5	ng	320399	6	15.527	849606	20.0
Triacontanal	16.774	4.3	ng	182909	6	15.527	849606	20.0
1,4-Dimethyl-8-...	17.174	27.1	ng	1148910	6	15.527	849606	20.0
(-)-Isolongifol...	17.515	4.1	ng	173110	6	15.527	849606	20.0
.gamma.-Sitosterol	17.627	6.3	ng	267070	6	15.527	849606	20.0
Androst-4-en-3-...	18.639	6.4	ng	272804	6	15.527	849606	20.0