LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033125\
Data File : BF142195.D
Acq On : 31 Mar 2025 22:25
Operator : RC/JU
Sample : Q1674-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT5358

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-BF031025.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142195.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	7	15	rVB	818120	1261730	39.20%	5.523%
2	2.246	20	26	41	rVB	27104	50995	1.58%	0.223%
3	5.081	497	508	523	rBV	157764	256610	7.97%	1.123%
4	5.481	570	576	599	rBV	1757674	2345695	72.88%	10.267%
5	6.486	741	747	767	rBV	1680578	2349756	73.00%	10.285%
6	6.863	806	811	819	rBV	466970	584394	18.16%	2.558%
7	7.428	901	907	917	rBV	1153774	1557513	48.39%	6.817%
8	8.145	1024	1029	1047	rBV	553021	737963	22.93%	3.230%
9	9.222	1206	1212	1228	rBV	2566392	3218681	100.00%	14.088%
10	9.904	1322	1328	1342	rBV	597305	784994	24.39%	3.436%
11	10.616	1444	1449	1456	rBV	246784	317087	9.85%	1.388%
12	10.692	1456	1462	1477	rVV	1322315	1782397	55.38%	7.801%
13	11.392	1575	1581	1591	rBV	490620	735330	22.85%	3.219%
14	11.616	1613	1619	1627	rBV2	17878	44249	1.37%	0.194%
15	11.910	1662	1669	1682	rBV3	144241	289349	8.99%	1.266%
16	12.163	1708	1712	1716	rBV2	27950	40259	1.25%	0.176%
17	12.604	1782	1787	1792	rBV	174962	247919	7.70%	1.085%
18	12.698	1799	1803	1808	rBV2	40996	69311	2.15%	0.303%
19	12.833	1820	1826	1830	rBV2	100468	151818	4.72%	0.665%
20	12.974	1844	1850	1858	rBV	2082918	2653208	82.43%	11.613%
21	13.668	1964	1968	1977	rVB2	34300	50096	1.56%	0.219%
22	13.874	1998	2003	2014	rVB3	109803	222718	6.92%	0.975%
23	14.027	2023	2029	2044	rVB2	518014	863422	26.83%	3.779%
24	14.504	2106	2110	2122	rBV5	36299	96268	2.99%	0.421%
25	14.657	2132	2136	2141	rBV	49072	67921	2.11%	0.297%
26	14.951	2182	2186	2190	rVB	62157	79075	2.46%	0.346%
27	15.074	2202	2207	2215	rBV	90953	197540	6.14%	0.865%
28	15.145	2215	2219	2221	rBV	49833	71165	2.21%	0.311%
29	15.380	2255	2259	2265	rVB	47274	72818	2.26%	0.319%
30	15.445	2266	2270	2275	rVV	33469	53981	1.68%	0.236%
31	15.509	2275	2281	2294	rVB	467700	797241	24.77%	3.489%
32	15.733	2315	2319	2326	rVB3	34060	58322	1.81%	0.255%
33	15.974	2354	2360	2365	rBV	75708	136381	4.24%	0.597%
34	16.033	2366	2370	2378	rVV10	16835	44817	1.39%	0.196%
35	16.786	2493	2498	2504	rBV3	32581	64844	2.01%	0.284%
36	16.992	2529	2533	2544	rBV2	19917	51482	1.60%	0.225%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033125\
Data File : BF142195.D
Acq On : 31 Mar 2025 22:25
Operator : RC/JU
Sample : Q1674-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT5358

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-BF031025.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.092	2545	2550	2557	rVB2	29719	64637	2.01%	0.283%
38	17.180	2560	2565	2579	rBV2	19800	75912	2.36%	0.332%
39	17.439	2606	2609	2617	rVB2	18543	40889	1.27%	0.179%
40	17.592	2628	2635	2657	rBV2	49578	211699	6.58%	0.927%
41	18.245	2742	2746	2754	rVB8	19487	46445	1.44%	0.203%

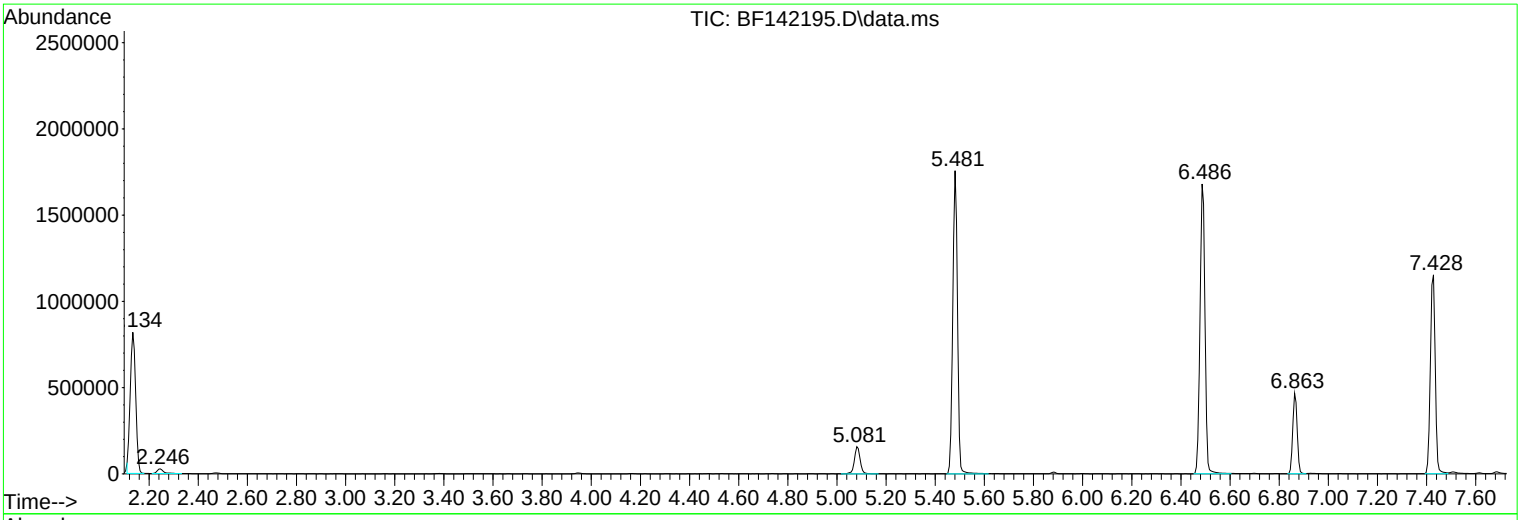
Sum of corrected areas: 22846931

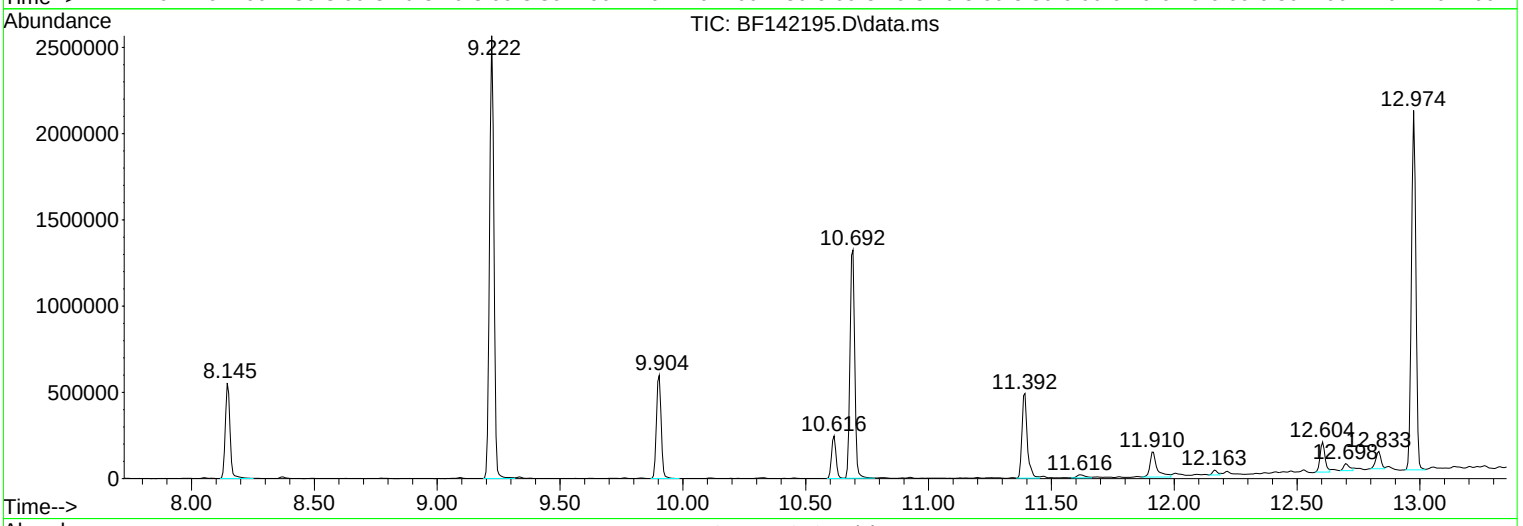
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033125\
Data File : BF142195.D
Acq On : 31 Mar 2025 22:25
Operator : RC/JU
Sample : Q1674-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

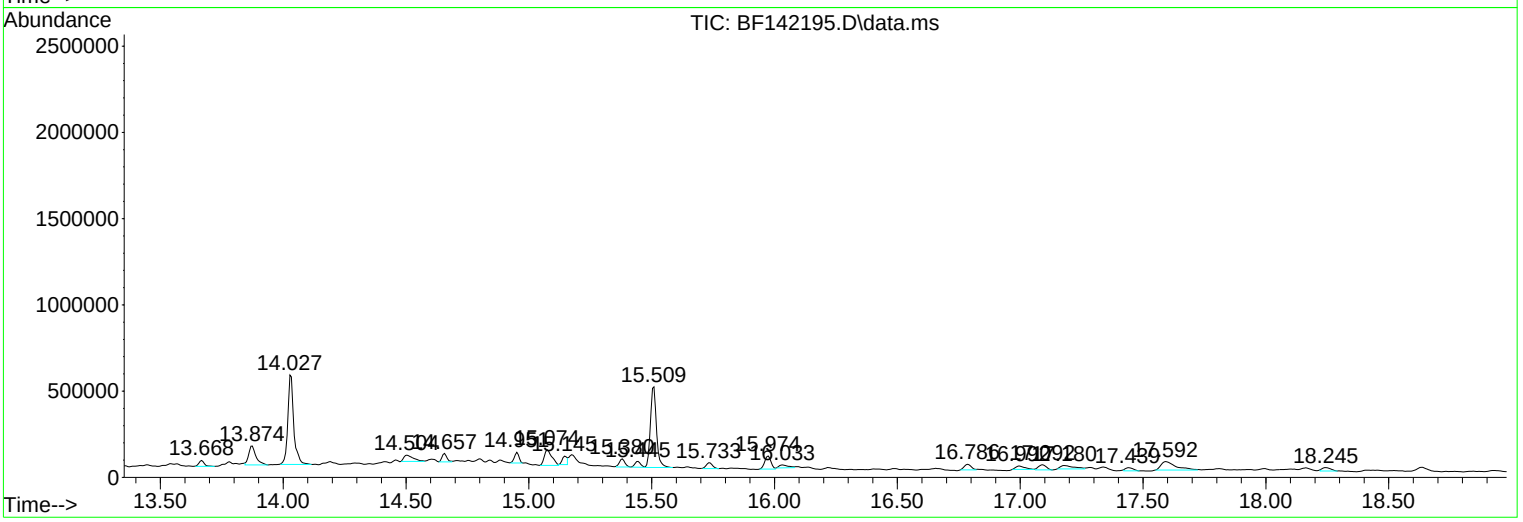
Instrument :
BNA_F
ClientSampleId :
RT5358

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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\BF033125\
Data File : BF142195.D
Acq On : 31 Mar 2025 22:25
Operator : RC/JU
Sample : Q1674-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT5358

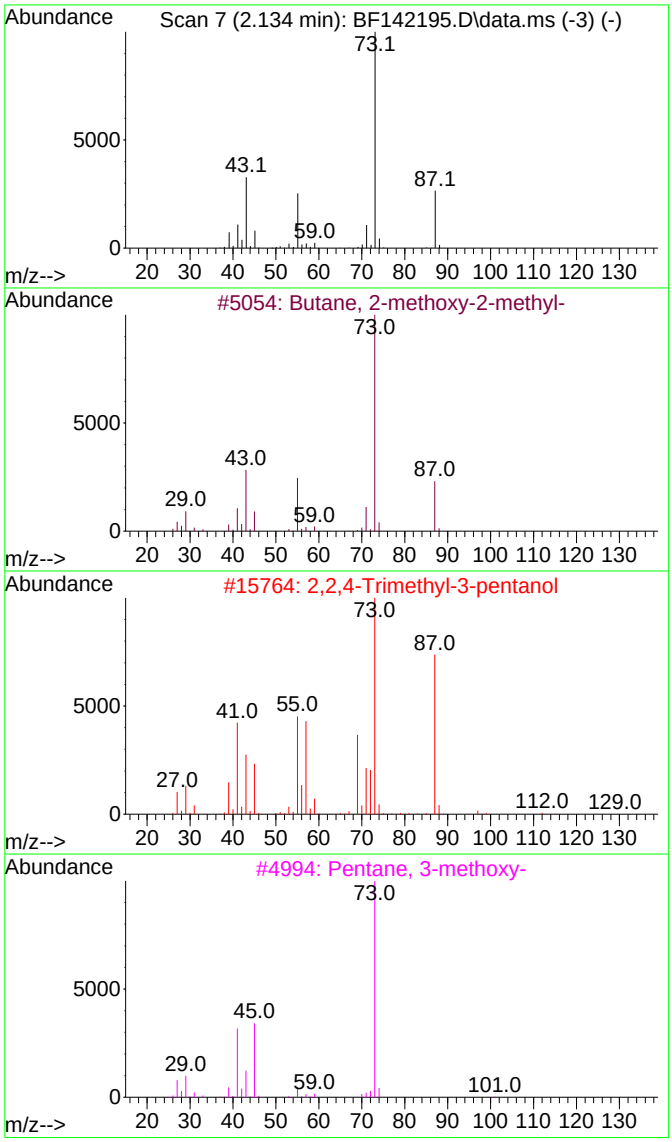
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

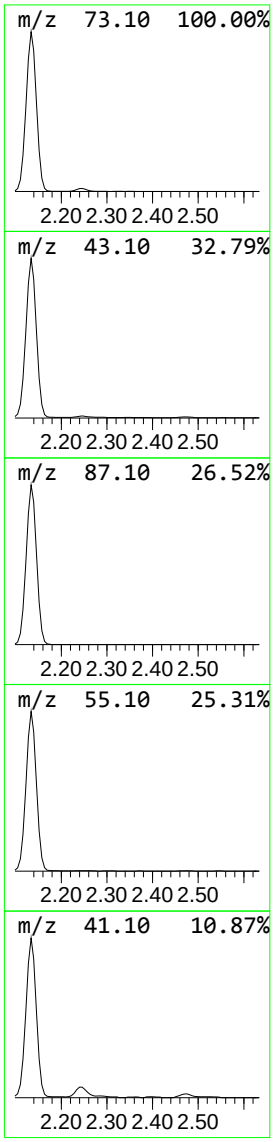
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	43.18 ng	1261730	1,4-Dichlorobenzene-d4	6.863

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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033125\
Data File : BF142195.D
Acq On : 31 Mar 2025 22:25
Operator : RC/JU
Sample : Q1674-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT5358

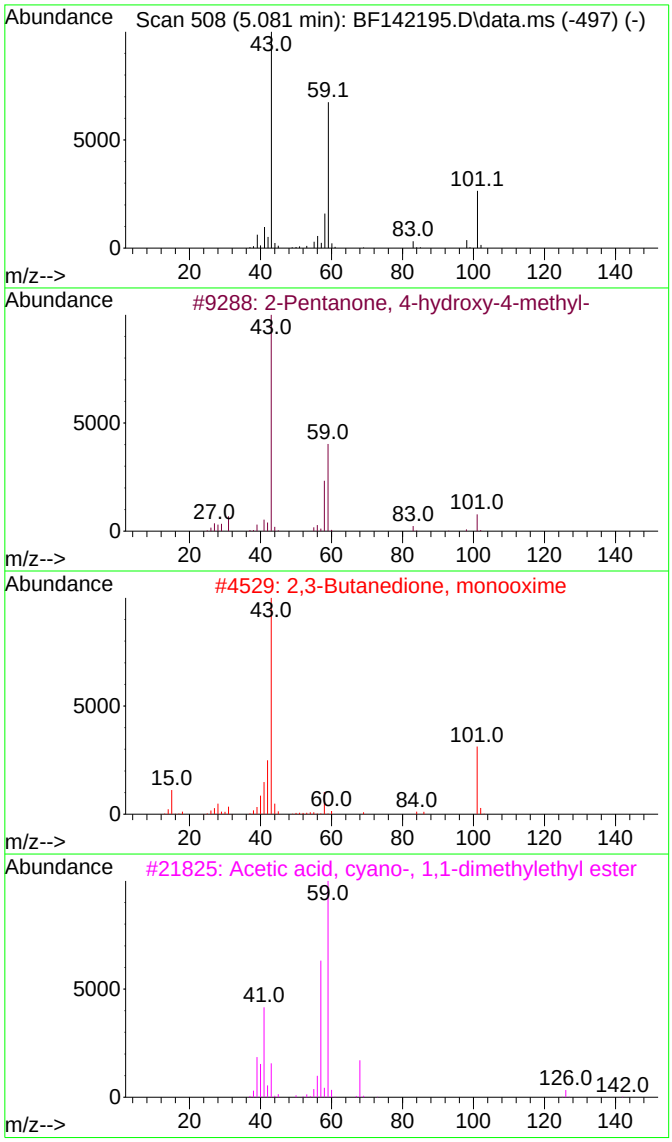
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

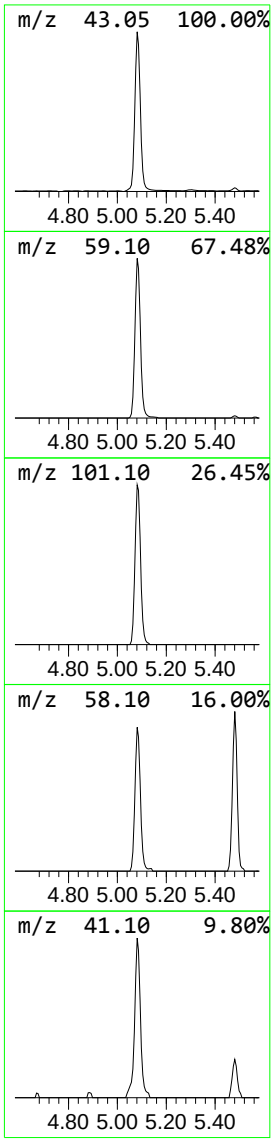
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	8.78 ng	256610	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Acetone	58	C3H6O	000067-64-1	10
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033125\
Data File : BF142195.D
Acq On : 31 Mar 2025 22:25
Operator : RC/JU
Sample : Q1674-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT5358

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

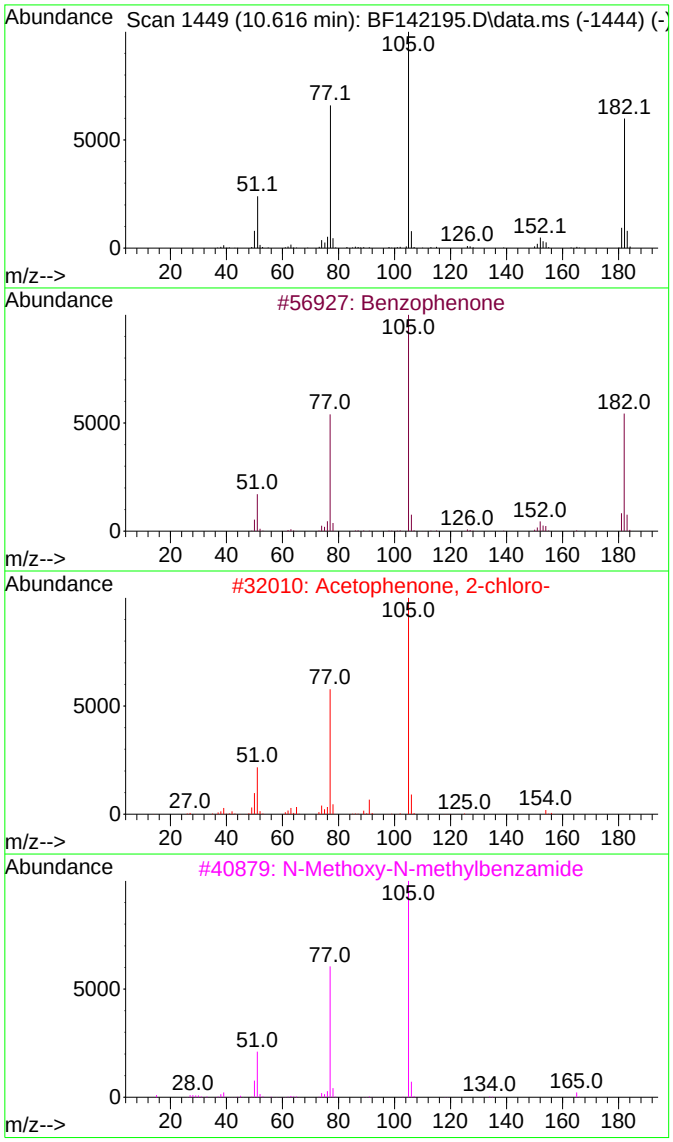
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

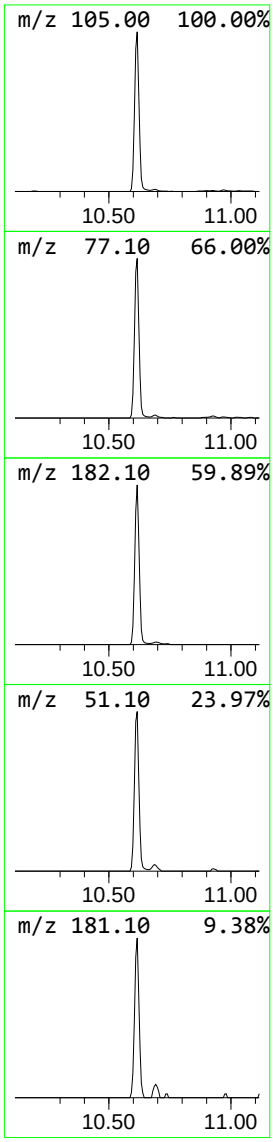
****

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.616	8.08 ng	317087	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
4	N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47
5	Vinyl benzoate	148	C9H8O2	000769-78-8	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033125\
Data File : BF142195.D
Acq On : 31 Mar 2025 22:25
Operator : RC/JU
Sample : Q1674-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT5358

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

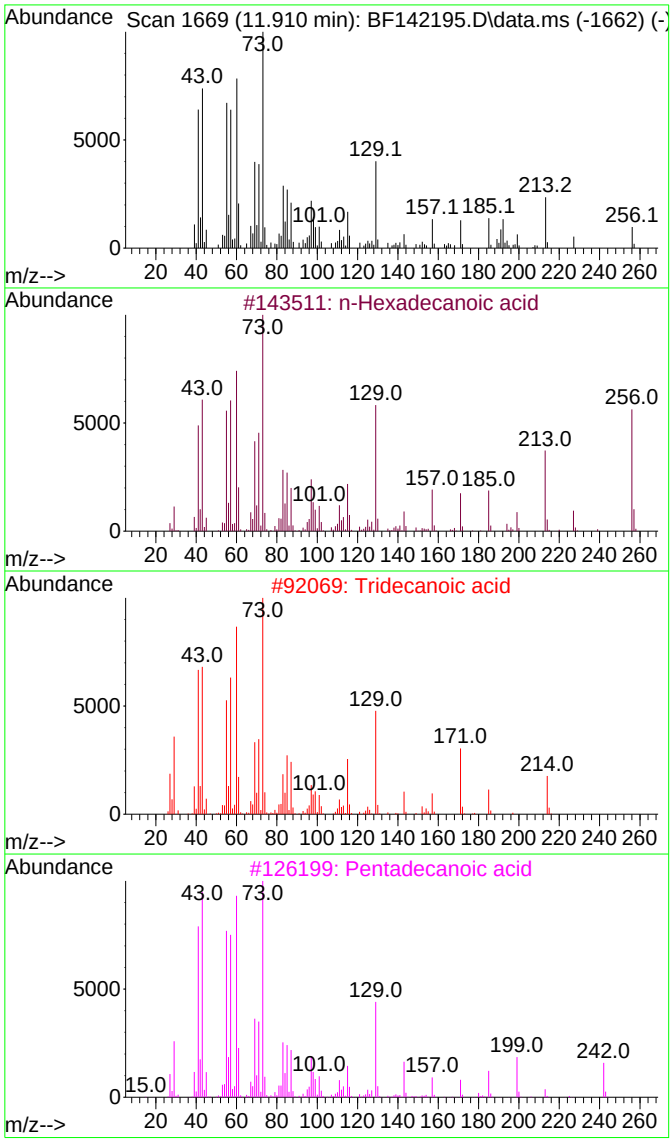
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

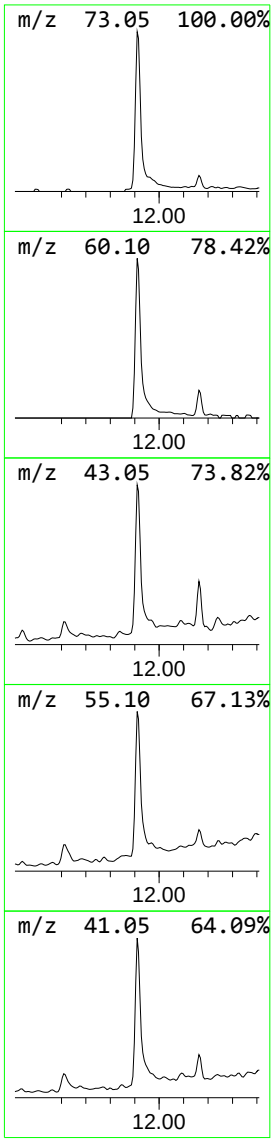
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	7.87 ng	289349	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	55





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033125\
Data File : BF142195.D
Acq On : 31 Mar 2025 22:25
Operator : RC/JU
Sample : Q1674-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT5358

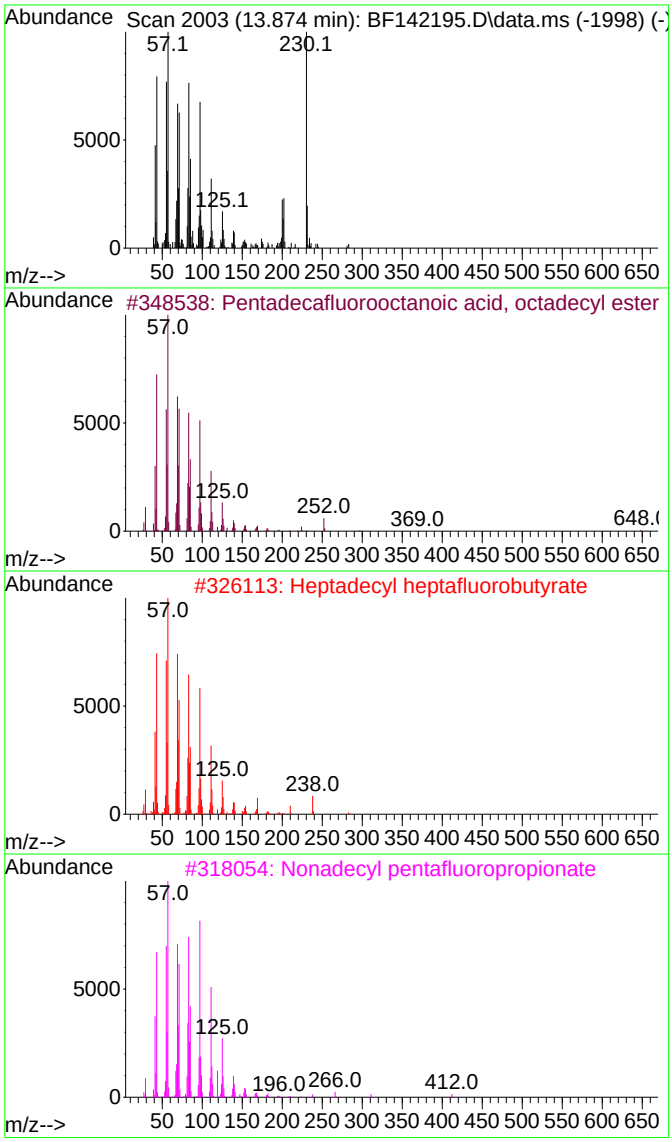
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

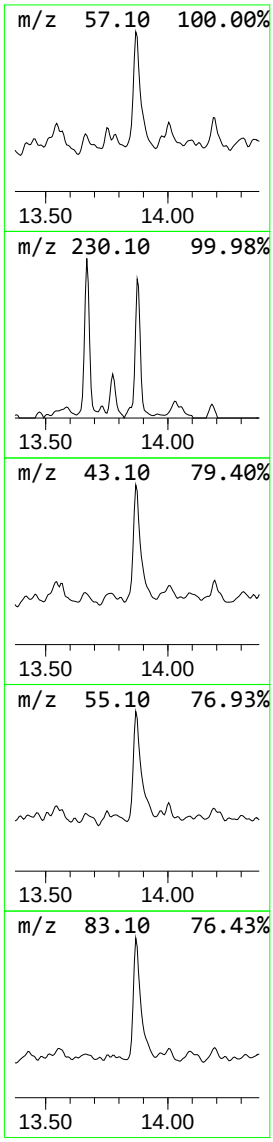
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	5.16 ng	222718	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	86
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	78
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	60
4	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	55
5	Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033125\
Data File : BF142195.D
Acq On : 31 Mar 2025 22:25
Operator : RC/JU
Sample : Q1674-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT5358

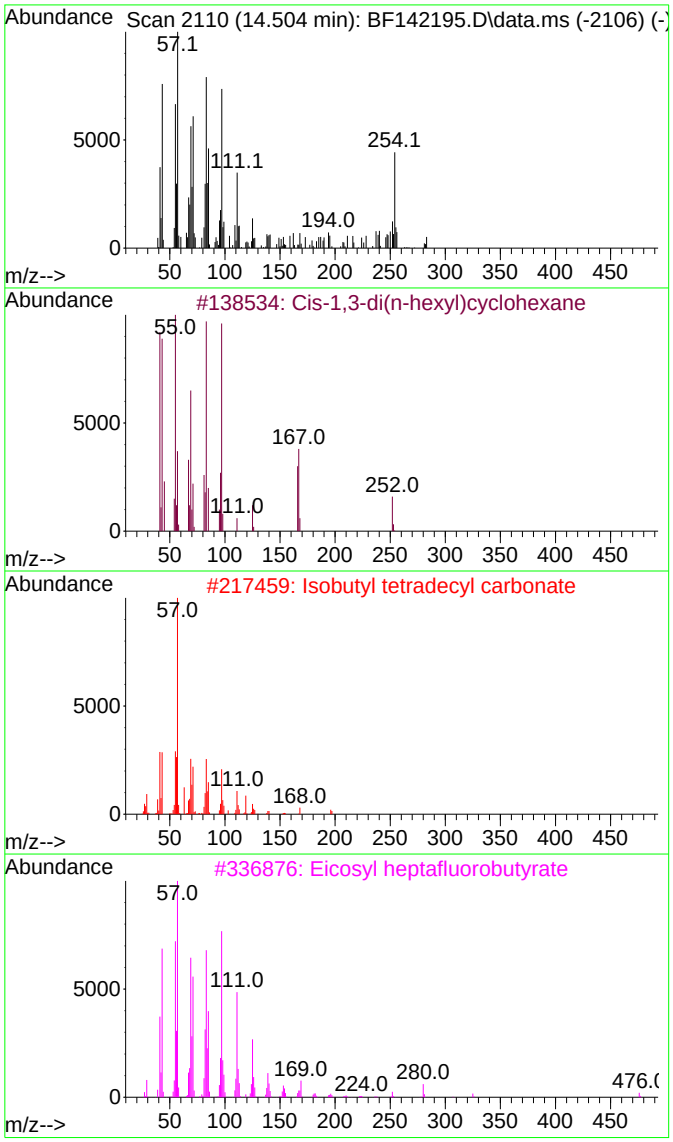
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

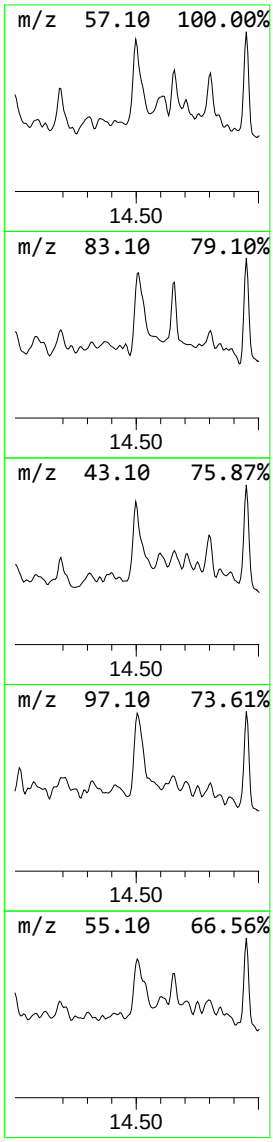
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cis-1,3-di(n-hexyl)cyclohexane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.504	2.23 ng	96268	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cis-1,3-di(n-hexyl)cyclohexane	252	C18H36	086701-17-9	90
2	Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	74
3	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	68
4	Cyclohexadecane	224	C16H32	000295-65-8	64
5	Cetene	224	C16H32	000629-73-2	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033125\
Data File : BF142195.D
Acq On : 31 Mar 2025 22:25
Operator : RC/JU
Sample : Q1674-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT5358

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

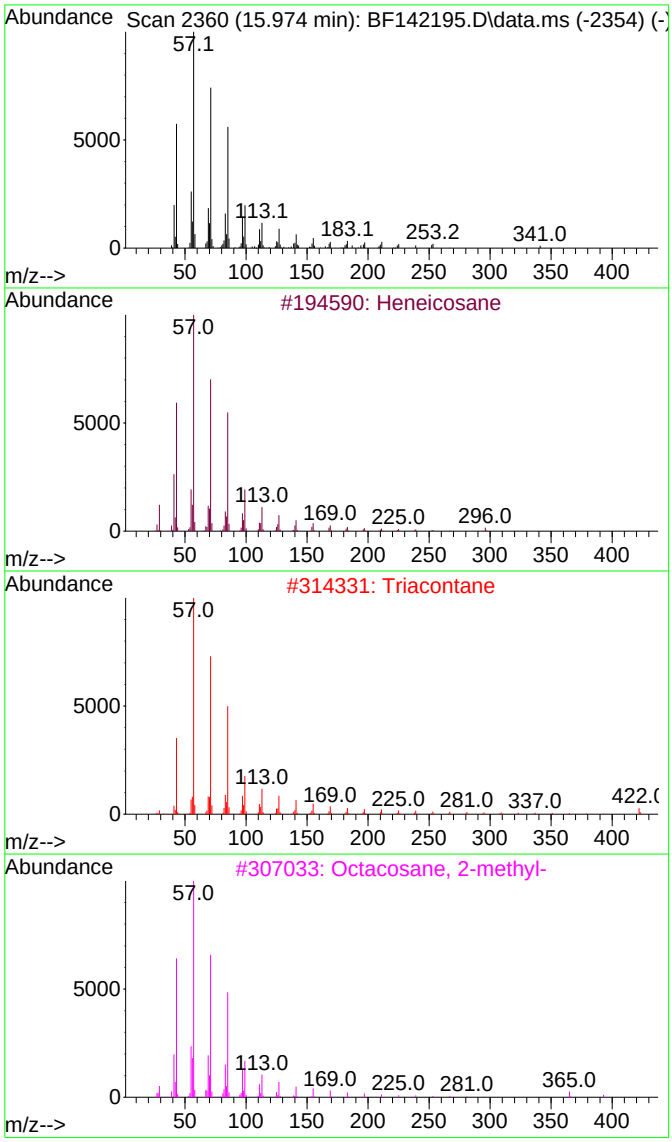
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

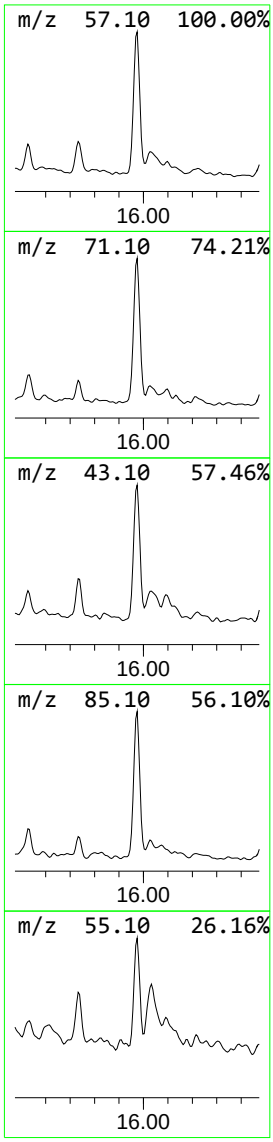
****

Peak Number 7 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.974	3.42 ng	136381	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Triacontane	422	C30H62	000638-68-6	91
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033125\
Data File : BF142195.D
Acq On : 31 Mar 2025 22:25
Operator : RC/JU
Sample : Q1674-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT5358

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

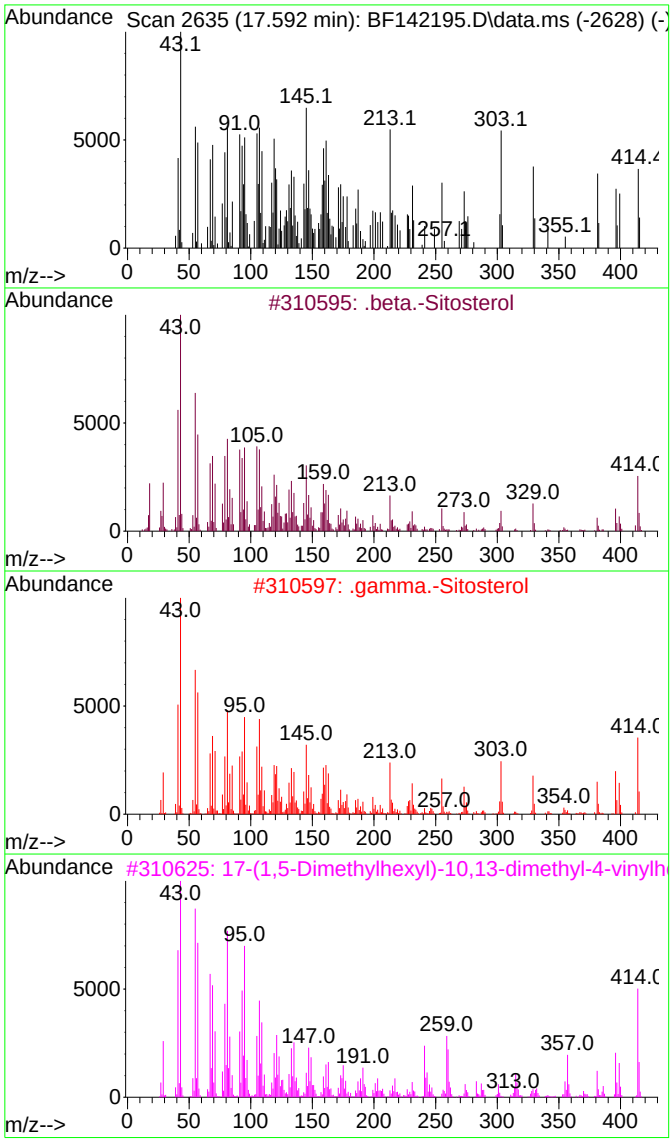
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

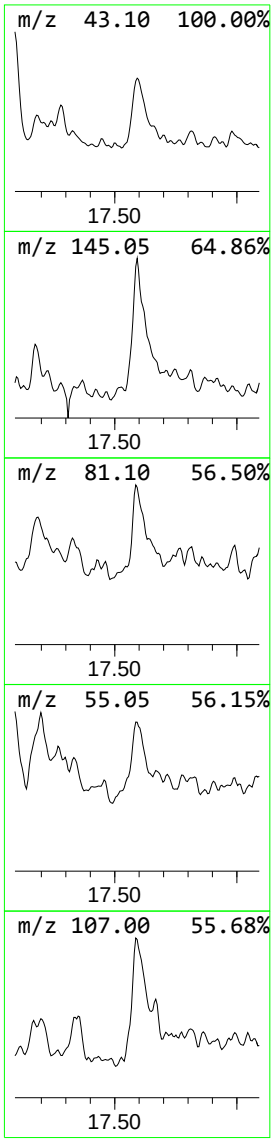
****

Peak Number 8 .beta.-Sitosterol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.592	5.31 ng	211699	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol	414	C29H50O	000083-46-5	96
2	.gamma.-Sitosterol	414	C29H50O	000083-47-6	60
3	17-(1,5-Dimethylhexyl)-10,13-dim...	414	C29H50O	1000210-86-9	25
4	(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	18
5	Benzopyrazine, 1,2,3,4-tetrahydr...	303	C16H21N3O3	342390-29-8	18





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033125\
Data File : BF142195.D
Acq On : 31 Mar 2025 22:25
Operator : RC/JU
Sample : Q1674-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT5358

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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...	2.134	43.2	ng	1261730	1	6.863	584394	20.0
2-Pentanone, 4-...	5.081	8.8	ng	256610	1	6.863	584394	20.0
Benzophenone	10.616	8.1	ng	317087	3	9.904	784994	20.0
n-Hexadecanoic ...	11.910	7.9	ng	289349	4	11.392	735330	20.0
Pentadecafluoro...	13.874	5.2	ng	222718	5	14.027	863422	20.0
Cis-1,3-di(n-he...	14.504	2.2	ng	96268	5	14.027	863422	20.0
Heneicosane	15.974	3.4	ng	136381	6	15.509	797241	20.0
.beta.-Sitosterol	17.592	5.3	ng	211699	6	15.509	797241	20.0