LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129407.D
Acq On : 28 Jul 2022 14:08
Operator : CG\JU
Sample : N3894-17
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RVE-36

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: BF129407.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.110	477	480	493	rVB	112193	138602	2.65%	0.415%
2	5.510	544	548	551	rBV	3638657	3152292	60.29%	9.440%
3	6.516	715	719	722	rBV	3308378	3279008	62.71%	9.819%
4	6.881	778	781	785	rBV	1327866	1057142	20.22%	3.166%
5	7.445	872	877	880	rBV	2537351	2321070	44.39%	6.951%
6	8.163	996	999	1003	rBV	1566435	1379490	26.38%	4.131%
7	9.239	1178	1182	1186	rBV	4525577	4139097	79.16%	12.395%
8	9.922	1294	1298	1302	rBV	1699376	1461538	27.95%	4.377%
9	10.716	1429	1433	1436	rBV	2251883	1917770	36.68%	5.743%
10	11.416	1548	1552	1555	rBV	1405312	1199341	22.94%	3.591%
11	11.933	1637	1640	1644	rBV3	61388	55407	1.06%	0.166%
12	12.492	1731	1735	1745	rVB5	28852	59483	1.14%	0.178%
13	12.998	1817	1821	1824	rBV	3058686	2578212	49.31%	7.721%
14	13.563	1913	1917	1927	rVB	169761	177499	3.39%	0.532%
15	13.910	1969	1976	1986	rBV2	150725	413647	7.91%	1.239%
16	14.057	1997	2001	2005	rBV	1000074	871288	16.66%	2.609%
17	14.510	2075	2078	2081	rBV	65497	63619	1.22%	0.191%
18	15.162	2186	2189	2193	rVB	99620	106087	2.03%	0.318%
19	15.551	2250	2255	2265	rVB	897934	1121492	21.45%	3.358%
20	15.762	2288	2291	2295	rBV5	37505	55176	1.06%	0.165%
21	15.998	2327	2331	2337	rVB	106610	152208	2.91%	0.456%
22	17.227	2531	2540	2553	rBV	2398786	5228777	100.00%	15.658%
23	17.562	2591	2597	2608	rVB3	347687	754881	14.44%	2.261%
24	18.074	2677	2684	2694	rVB5	278277	686330	13.13%	2.055%
25	18.433	2738	2745	2756	rVB	392048	1024668	19.60%	3.068%

Sum of corrected areas: 33394124

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Misc :
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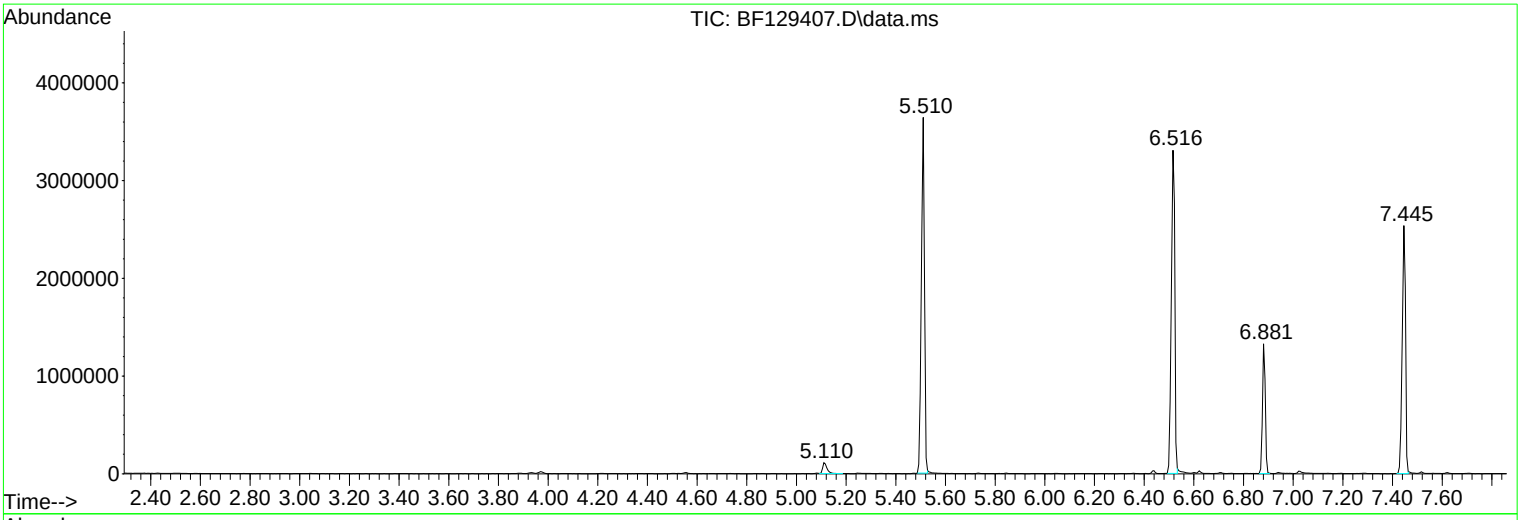
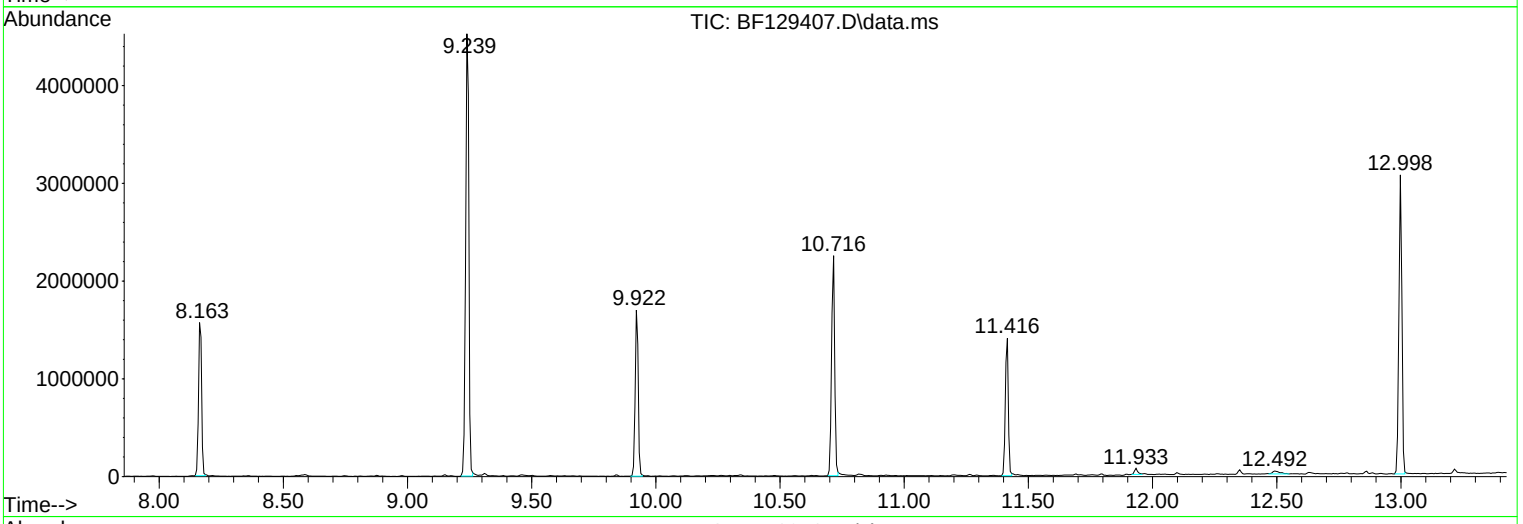
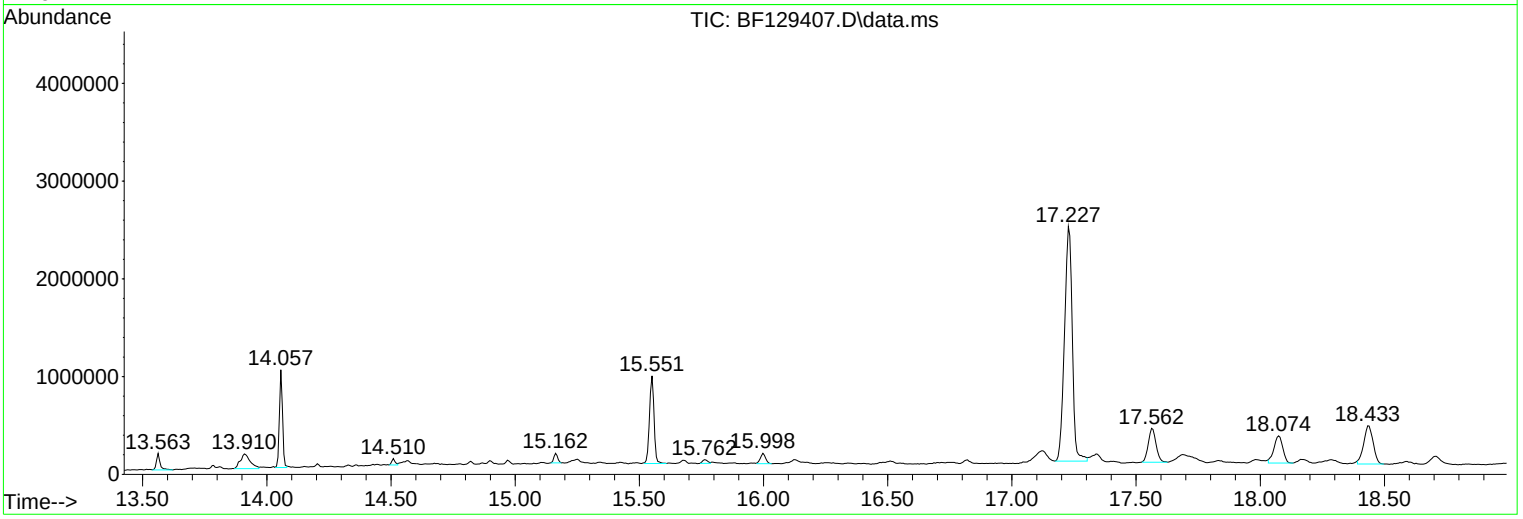
Instrument :
BNA_F
ClientSampleId :
RVE-36

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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Data File : BF129407.D
Acq On : 28 Jul 2022 14:08
Operator : CG\JU
Sample : N3894-17
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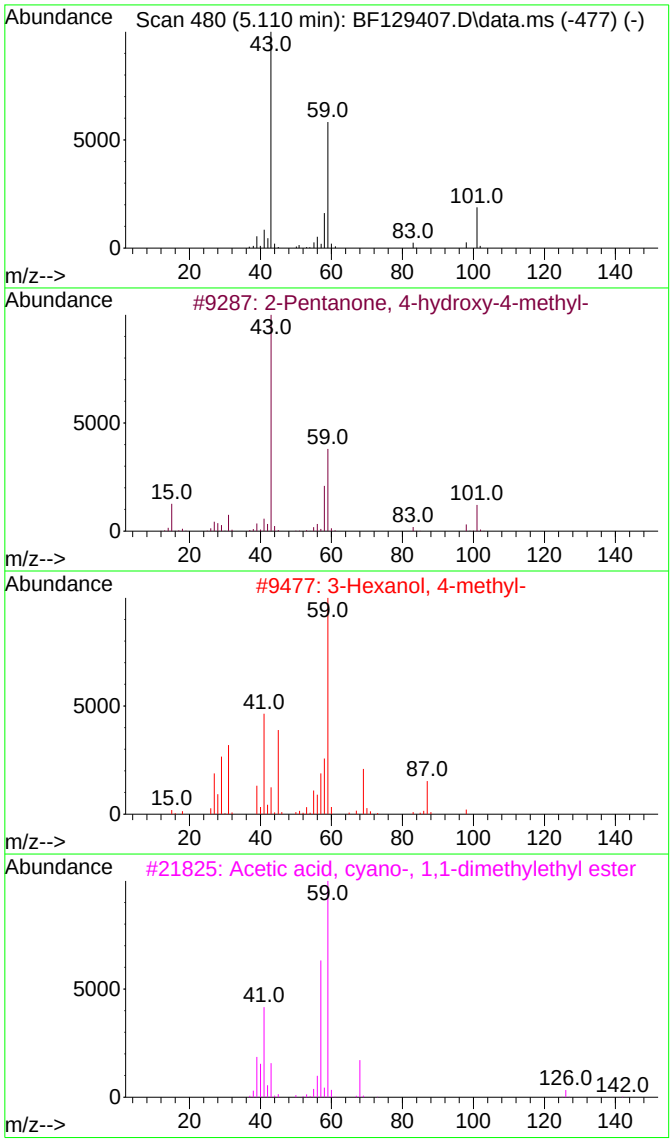
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

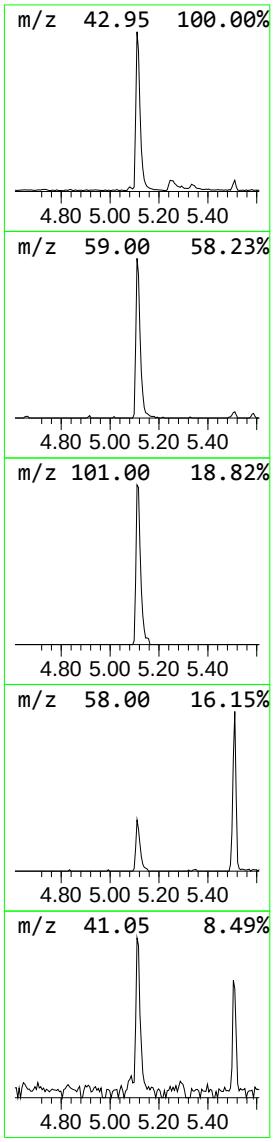
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	2.62 ng	138602	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





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Data File : BF129407.D
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Operator : CG\JU
Sample : N3894-17
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-36

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
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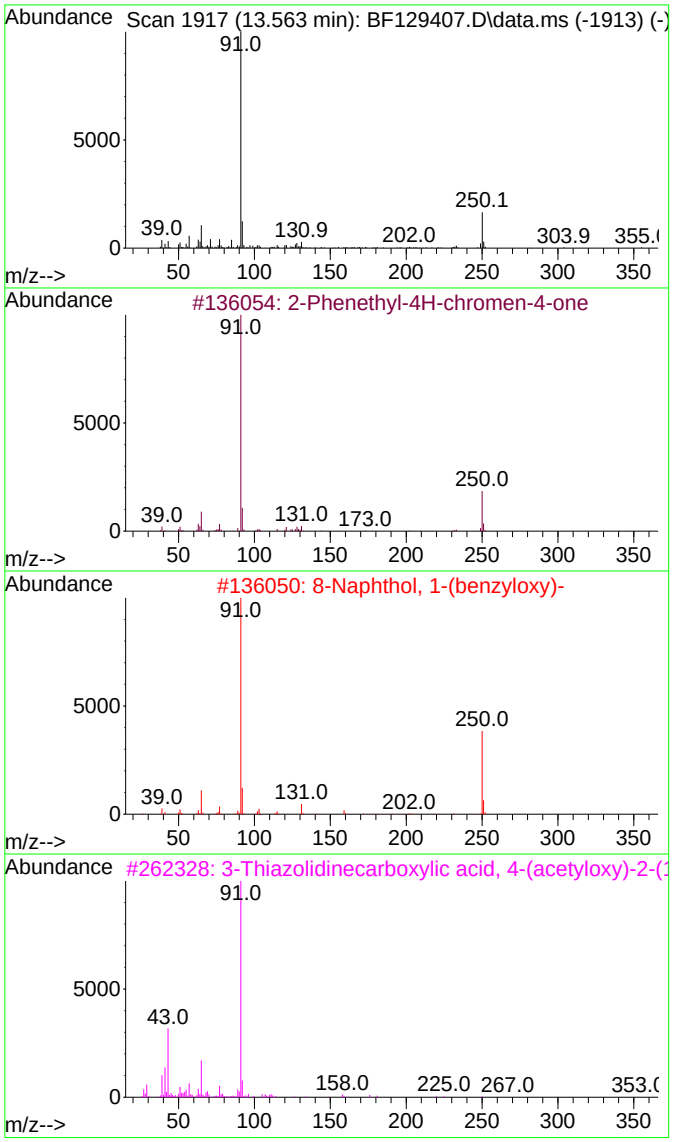
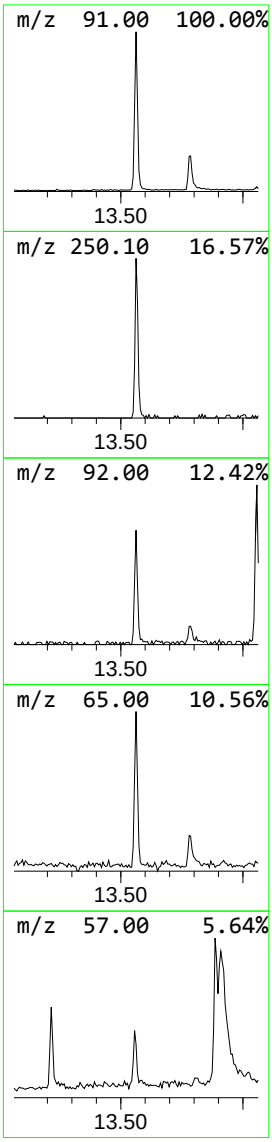
****
Peak Number 2 2-Phenethyl-4H-chromen-4-one Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.563	4.07 ng	177499	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenethyl-4H-chromen-4-one	250	C17H14O2	061828-53-3	96
2	8-Naphthol, 1-(benzyloxy)-	250	C17H14O2	326875-68-7	68
3	3-Thiazolidinecarboxylic acid, 4...	353	C17H23NO5S	126990-62-3	50
4	1,6-Naphthyridin-4(1H)-one, 1-be...	304	C16H11F3N2O	161014-24-0	49
5	4H-1,2,4-triazol-3-ol, 5-[(pheny...	207	C9H9N3OS	1010400-54-3	47





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Operator : CG\JU
Sample : N3894-17
Misc :
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Instrument :
BNA_F
ClientSampleId :
RVE-36

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
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TIC Library : C:\Database\NIST20.L
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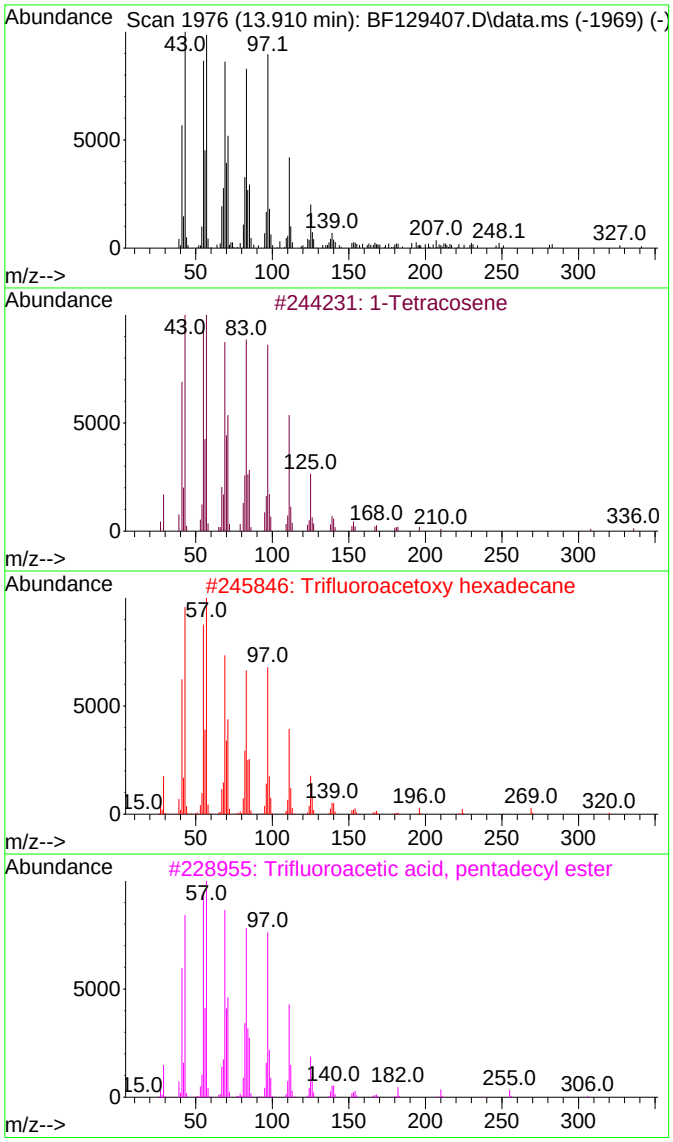
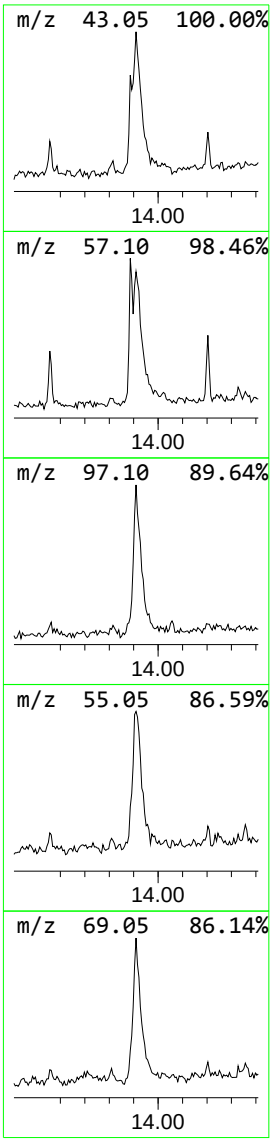
****

Peak Number 3 1-Tetracosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	9.50 ng	413647	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4	1-Hexacosene	364	C26H52	018835-33-1	94
5	Behenic alcohol	326	C22H46O	000661-19-8	94





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Acq On : 28 Jul 2022 14:08
Operator : CG\JU
Sample : N3894-17
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Instrument :
BNA_F
ClientSampleId :
RVE-36

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

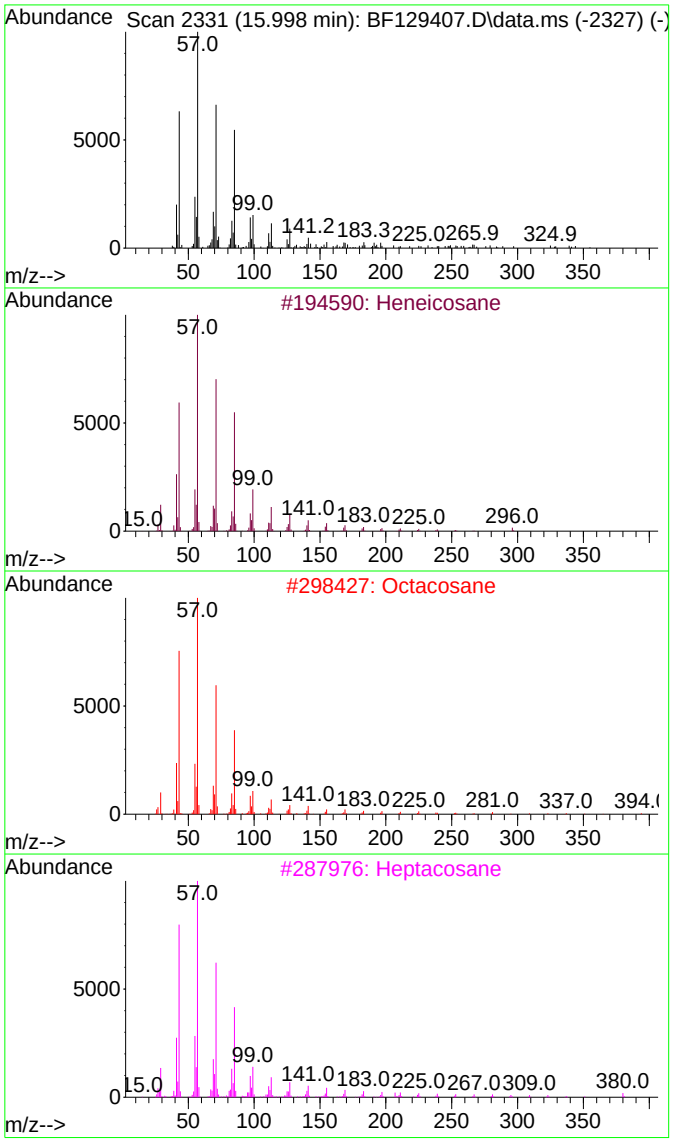
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

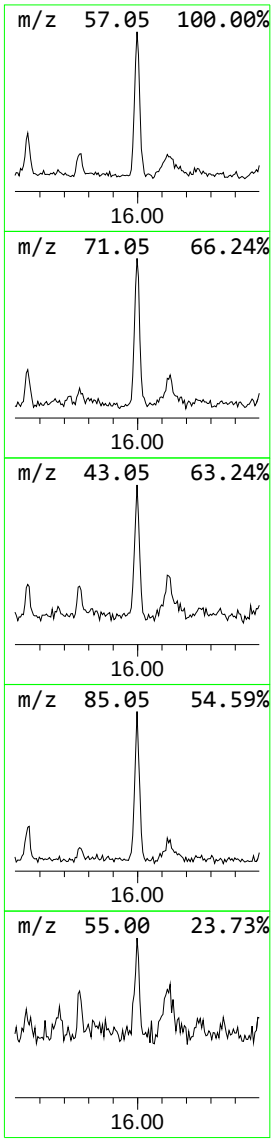
****

Peak Number 4 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.998	2.71 ng	152208	Perylene-d12	15.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Octacosane	394	C28H58	000630-02-4	87
3	Heptacosane	380	C27H56	000593-49-7	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87





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Operator : CG\JU
Sample : N3894-17
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-36

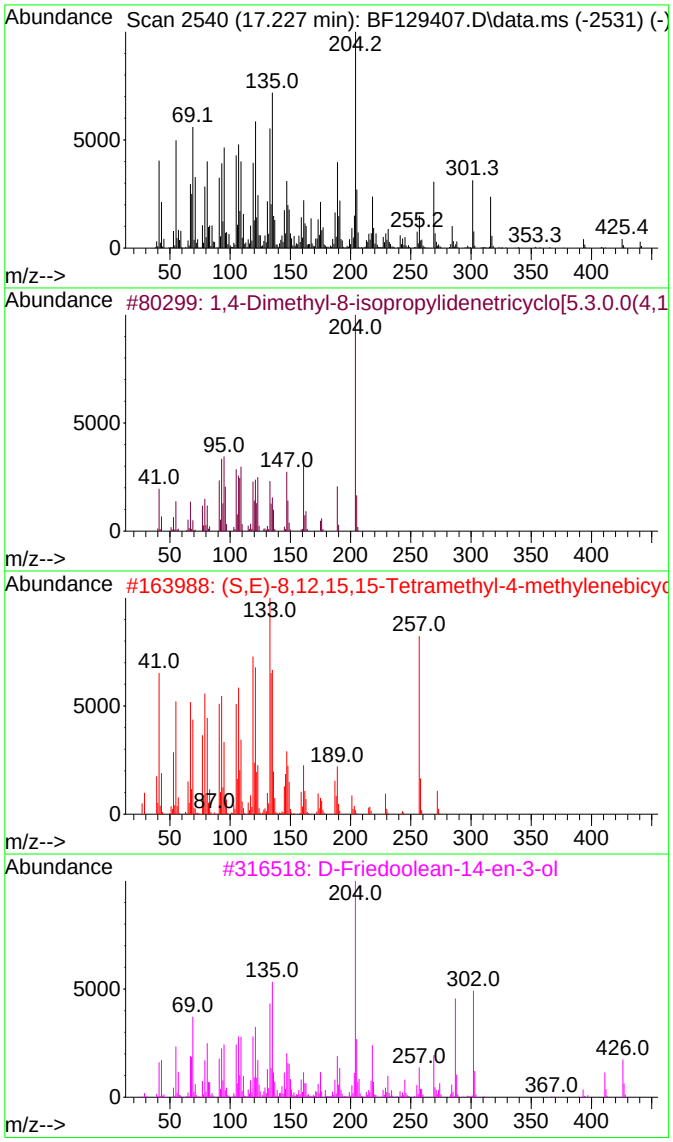
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

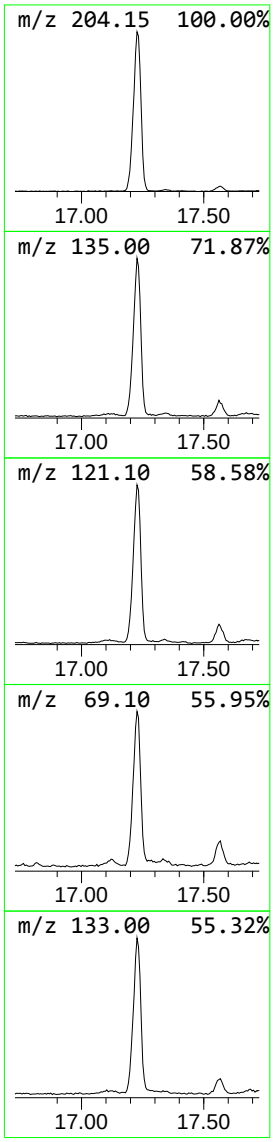
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1,4-Dimethyl-8-isopropylide... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.227	93.25 ng	5228780	Perylene-d12	15.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1010140-07-7	64
2	(S,E)-8,12,15,15-Tetramethyl-4-m...	272	C20H32	386223-19-4	60
3	D-Friedoolean-14-en-3-ol	426	C30H50O	081654-73-1	58
4	Farnesyl bromide	284	C15H25Br	006874-67-5	49
5	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	49





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Sample : N3894-17
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Instrument :
BNA_F
ClientSampleId :
RVE-36

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
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TIC Library : C:\Database\NIST20.L
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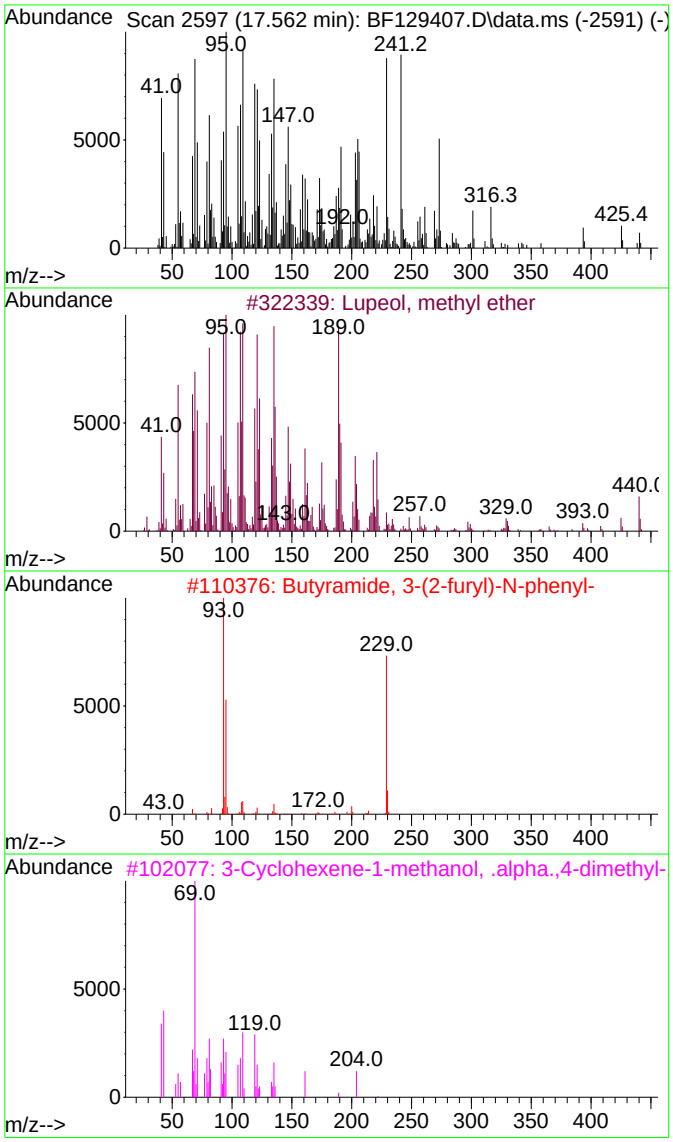
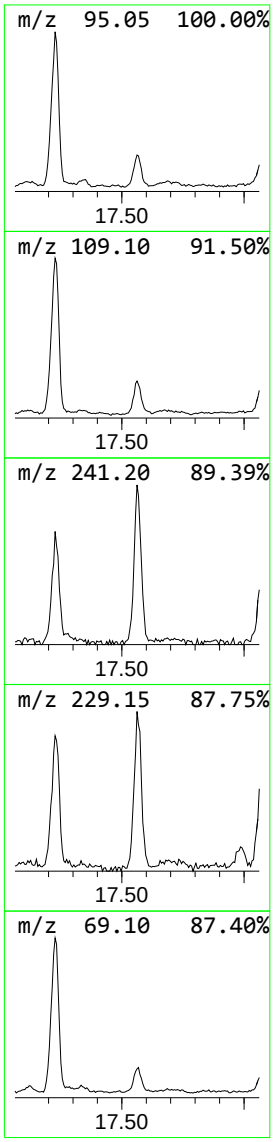
****

Peak Number 6 Lupeol, methyl ether Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.562	13.46 ng	754881	Perylene-d12	15.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lupeol, methyl ether	440	C31H52O	025279-38-3	70
2	Butyramide, 3-(2-furyl)-N-phenyl-	229	C14H15NO2	1000156-94-9	38
3	3-Cyclohexene-1-methanol, .alpha...	222	C15H26O	023178-88-3	30
4	2-Cyclohexene-1-carboxaldehyde, ...	220	C15H24O	056772-07-7	25
5	Tricyclo[4.3.0.0(7,9)]nonane, 2,...	206	C15H26	054832-82-5	25





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Operator : CG\JU
Sample : N3894-17
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-36

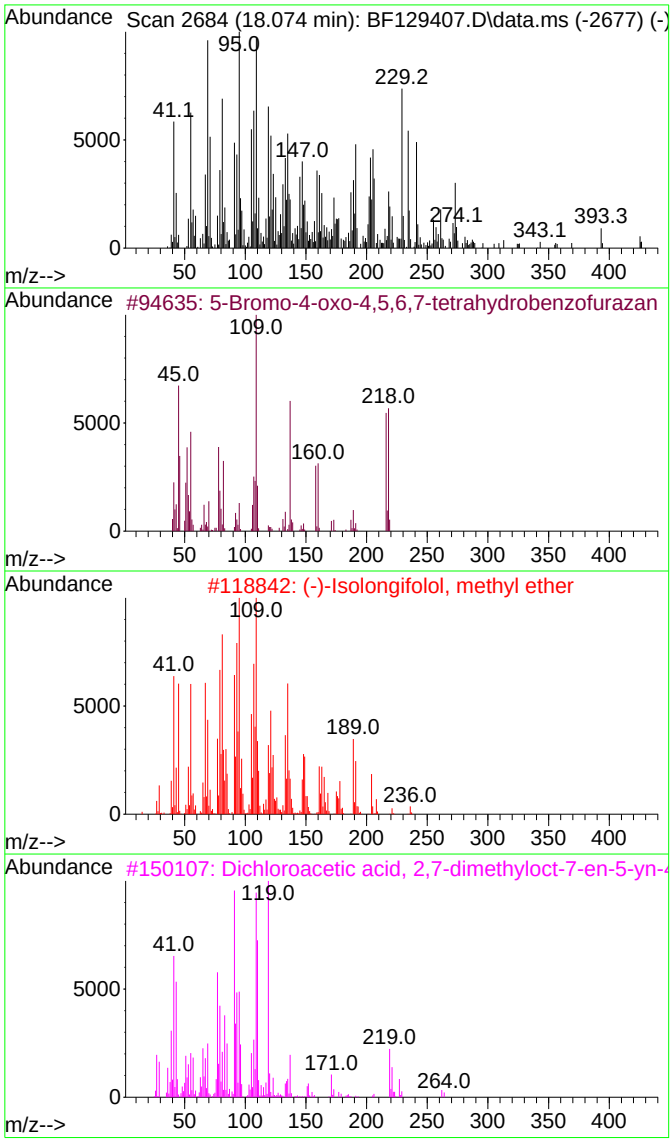
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

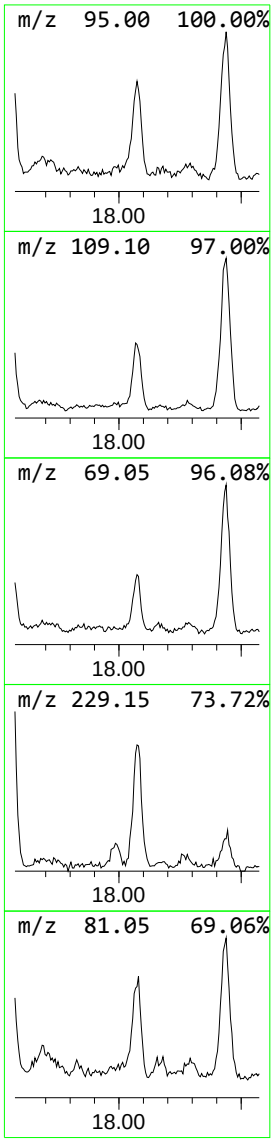
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 5-Bromo-4-oxo-4,5,6,7-tetra... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.074	12.24 ng	686330	Perylene-d12	15.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	90
2	(-)-Isolongifolol, methyl ether	236	C16H28O	1000333-80-8	50
3	Dichloroacetic acid, 2,7-dimethy...	262	C12H16Cl2O2	1000299-43-4	46
4	p-Camphorene	272	C20H32	020016-72-2	43
5	9-Thiabicyclo[3.3.1]nonane, 2,6-...	274	C14H18N4S	1000141-52-1	40





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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
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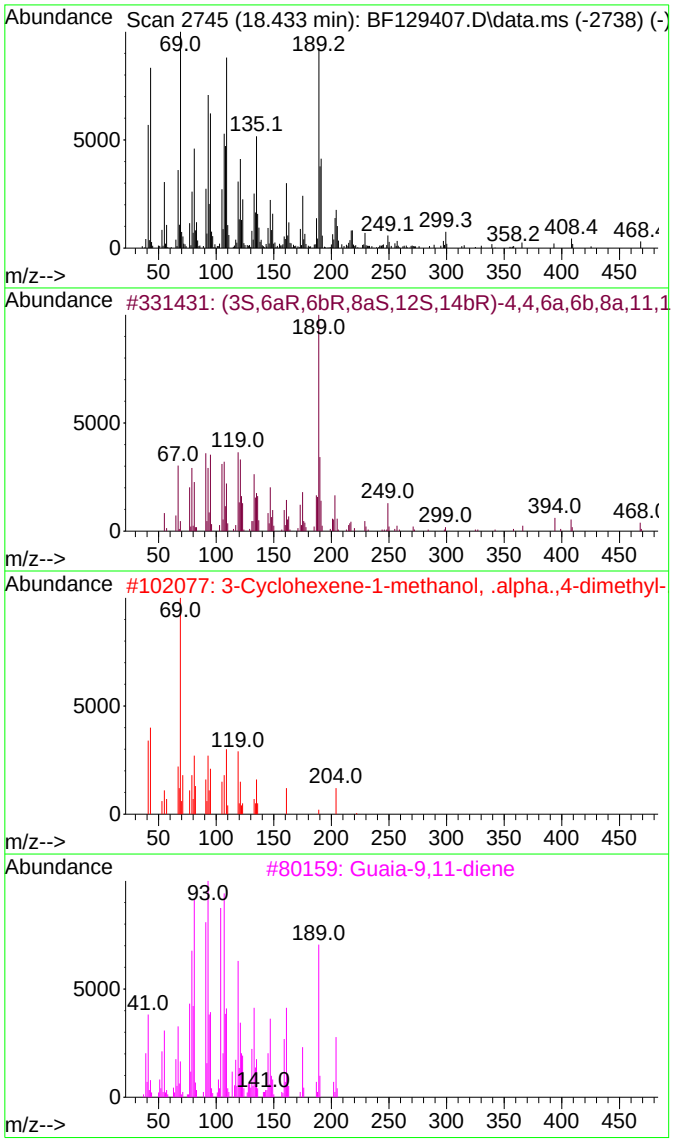
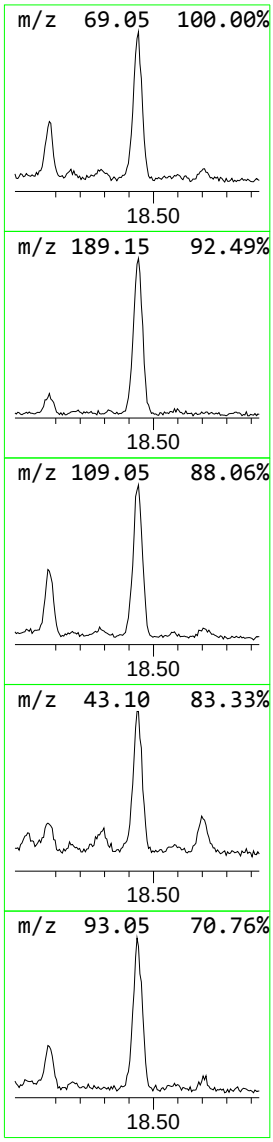
****

Peak Number 8 unknown18.433 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.433	18.27 ng	1024670	Perylene-d12	15.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3S,6aR,6bR,8aS,12S,14bR)-4,4,6a...	468	C32H52O2	1000441-99-9	49
2	3-Cyclohexene-1-methanol, .alpha...	222	C15H26O	023178-88-3	49
3	Guaia-9,11-diene	204	C15H24	1000374-19-8	42
4	Epilupeol; 20(29)-Lupen-3alpha-o...	468	C32H52O2	1010513-01-8	41
5	Levomenol	222	C15H26O	023089-26-1	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129407.D
Acq On : 28 Jul 2022 14:08
Operator : CG\JU
Sample : N3894-17
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-36

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
2-Pentanone, 4-...	5.110	2.6	ng	138602	1	6.881	1057140	20.0
2-Phenethyl-4H-...	13.563	4.1	ng	177499	5	14.057	871288	20.0
1-Tetracosene	13.910	9.5	ng	413647	5	14.057	871288	20.0
Heneicosane	15.998	2.7	ng	152208	6	15.551	1121490	20.0
1,4-Dimethyl-8-...	17.227	93.3	ng	5228780	6	15.551	1121490	20.0
Lupeol, methyl ...	17.562	13.5	ng	754881	6	15.551	1121490	20.0
5-Bromo-4-oxo-4...	18.074	12.2	ng	686330	6	15.551	1121490	20.0
unknown18.433	18.433	18.3	ng	1024670	6	15.551	1121490	20.0