LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090122\
Data File : BG054826.D
Acq On : 1 Sep 2022 17:37
Operator : CG/JU
Sample : N4439-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : KTS2-MH-02-0-20

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_G\Methods\8270-BG082522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054826.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.770	78	82	90	rBV	17867	27634	1.87%	0.190%
2	5.210	321	327	337	rVB	45829	79055	5.35%	0.544%
3	5.686	401	408	416	rBV	546395	881867	59.72%	6.073%
4	7.295	674	682	694	rBV	554180	953815	64.59%	6.569%
5	8.147	821	827	834	rBV	142246	238972	16.18%	1.646%
6	9.317	1019	1026	1039	rBV	315533	605582	41.01%	4.171%
7	9.881	1118	1122	1133	rVB9	8897	22204	1.50%	0.153%
8	9.998	1133	1142	1145	rBV9	9205	25564	1.73%	0.176%
9	10.039	1147	1149	1158	rVB3	11350	19559	1.32%	0.135%
10	10.139	1160	1166	1171	rBV6	12327	25917	1.76%	0.178%
11	10.668	1250	1256	1262	rBV10	9865	25851	1.75%	0.178%
12	10.973	1301	1308	1314	rBV	203011	355821	24.10%	2.450%
13	11.103	1325	1330	1336	rVB4	23214	38551	2.61%	0.265%
14	11.167	1337	1341	1346	rBV6	11290	21710	1.47%	0.150%
15	11.385	1374	1378	1383	rBV6	11866	21886	1.48%	0.151%
16	11.449	1384	1389	1394	rVB3	38979	64884	4.39%	0.447%
17	11.790	1442	1447	1450	rBV6	16546	31349	2.12%	0.216%
18	11.884	1457	1463	1469	rVB6	21937	48057	3.25%	0.331%
19	12.008	1480	1484	1488	rBV2	40206	64889	4.39%	0.447%
20	12.055	1488	1492	1500	rVB4	39576	75625	5.12%	0.521%
21	12.149	1504	1508	1514	rVB2	29822	47958	3.25%	0.330%
22	12.237	1518	1523	1534	rVB5	44118	98700	6.68%	0.680%
23	12.765	1609	1613	1617	rBV4	27125	56075	3.80%	0.386%
24	13.406	1716	1722	1732	rVB	773537	1219877	82.61%	8.401%
25	13.570	1745	1750	1757	rBV5	66692	164587	11.15%	1.133%
26	13.982	1815	1820	1825	rBV7	63962	134045	9.08%	0.923%
27	14.099	1836	1840	1845	rBV2	106428	152216	10.31%	1.048%
28	14.205	1854	1858	1866	rVB2	74200	184829	12.52%	1.273%
29	14.604	1923	1926	1931	rVB2	103314	152605	10.33%	1.051%
30	14.781	1952	1956	1963	rVB	319286	514962	34.87%	3.546%
31	15.562	2085	2089	2099	rVB3	100168	164596	11.15%	1.134%
32	16.267	2204	2209	2218	rBV	643960	958404	64.90%	6.600%
33	17.525	2418	2423	2428	rBV	391599	631954	42.79%	4.352%
34	19.622	2776	2780	2784	rVB	163101	218271	14.78%	1.503%
35	20.127	2861	2866	2871	rVB	1106196	1476709	100.00%	10.170%
36	20.768	2971	2975	2978	rBV	107325	155697	10.54%	1.072%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090122\
Data File : BG054826.D
Acq On : 1 Sep 2022 17:37
Operator : CG/JU
Sample : N4439-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
KTS2-MH-02-0-20

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_G\Methods\8270-BG082522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.803	2978	2981	2988	rVB3	111734	165815	11.23%	1.142%
38	21.426	3083	3087	3101	rVB	225331	357676	24.22%	2.463%
39	21.820	3148	3154	3160	rBV	360050	617536	41.82%	4.253%
40	24.193	3554	3558	3565	rVB2	66524	137432	9.31%	0.946%
41	25.186	3718	3727	3739	rVB2	234222	681552	46.15%	4.694%
42	26.925	4018	4023	4031	rVB5	47824	128658	8.71%	0.886%
43	27.025	4033	4040	4059	rVB10	66672	262099	17.75%	1.805%
44	27.578	4129	4134	4146	rVB9	75541	249977	16.93%	1.722%
45	30.139	4558	4570	4596	rVB7	150251	859769	58.22%	5.921%
46	30.932	4693	4705	4725	rVB8	191780	1038477	70.32%	7.152%
47	32.395	4948	4954	4955	rBV6	36113	61268	4.15%	0.422%

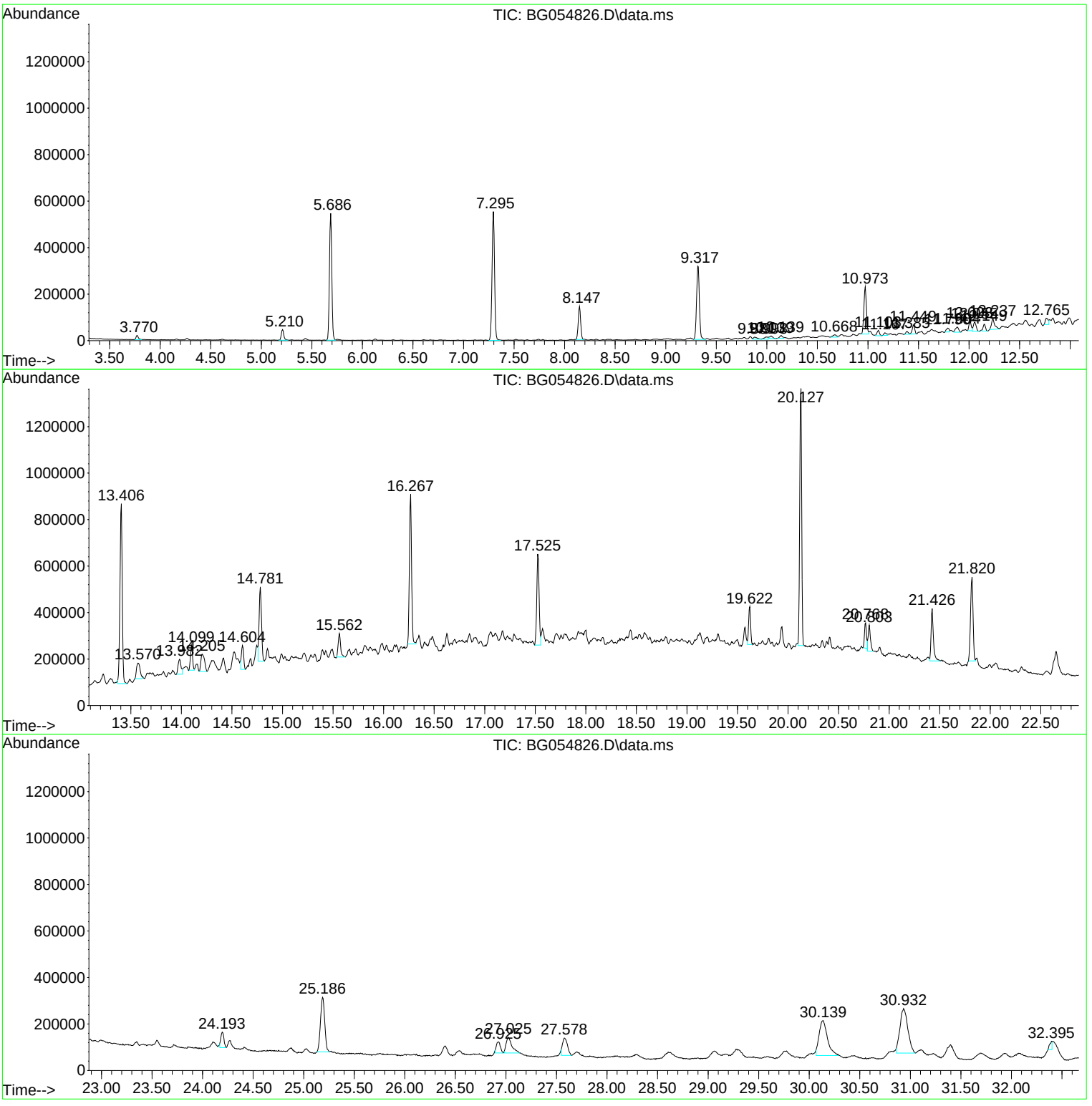
Sum of corrected areas: 14520536

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090122\
Data File : BG054826.D
Acq On : 1 Sep 2022 17:37
Operator : CG/JU
Sample : N4439-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
KTS2-MH-02-0-20

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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_G\Data\BG090122\
Data File : BG054826.D
Acq On : 1 Sep 2022 17:37
Operator : CG/JU
Sample : N4439-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
KTS2-MH-02-0-20

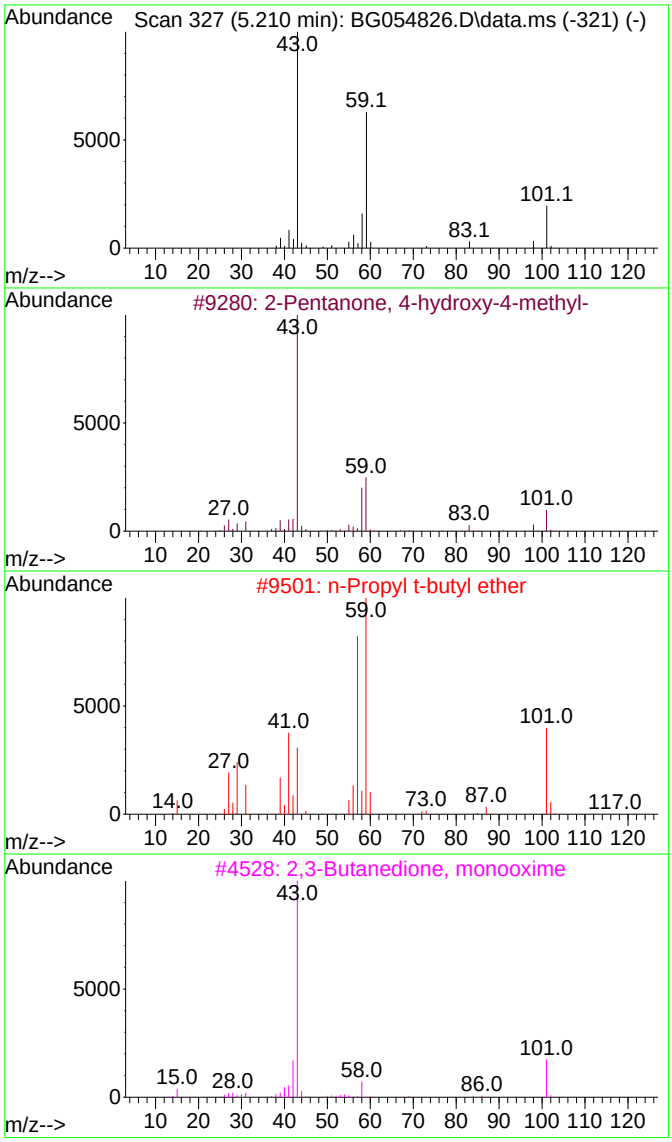
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

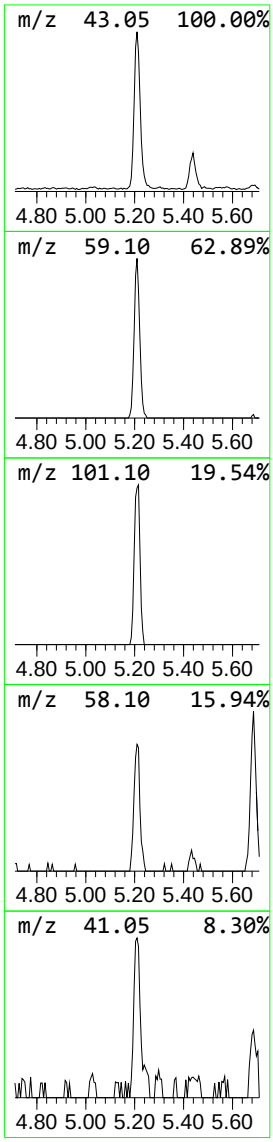
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.210	6.62 ng	79055	1,4-Dichlorobenzene-d4	8.147

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090122\
Data File : BG054826.D
Acq On : 1 Sep 2022 17:37
Operator : CG/JU
Sample : N4439-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
KTS2-MH-02-0-20

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

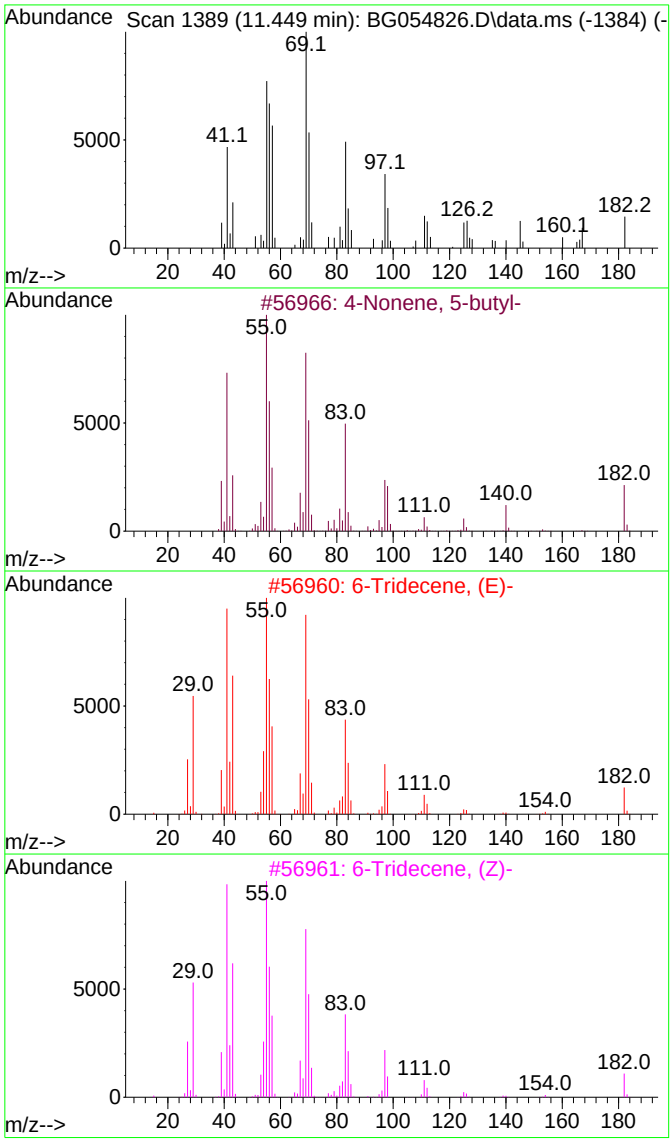
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

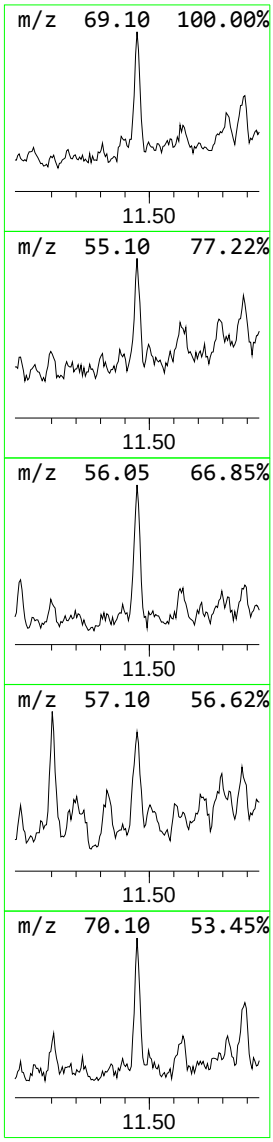
****

Peak Number 2 4-Nonene, 5-butyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.449	3.65 ng	64884	Naphthalene-d8	10.973

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Nonene, 5-butyl-	182	C13H26	007367-38-6	83
2	6-Tridecene, (E)-	182	C13H26	006434-76-0	83
3	6-Tridecene, (Z)-	182	C13H26	006508-77-6	83
4	Cyclohexane, 2-butyl-1,1,3-trime...	182	C13H26	054676-39-0	76
5	Cyclooctane, 1,2-dimethyl-	140	C10H20	013151-94-5	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090122\
Data File : BG054826.D
Acq On : 1 Sep 2022 17:37
Operator : CG/JU
Sample : N4439-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
KTS2-MH-02-0-20

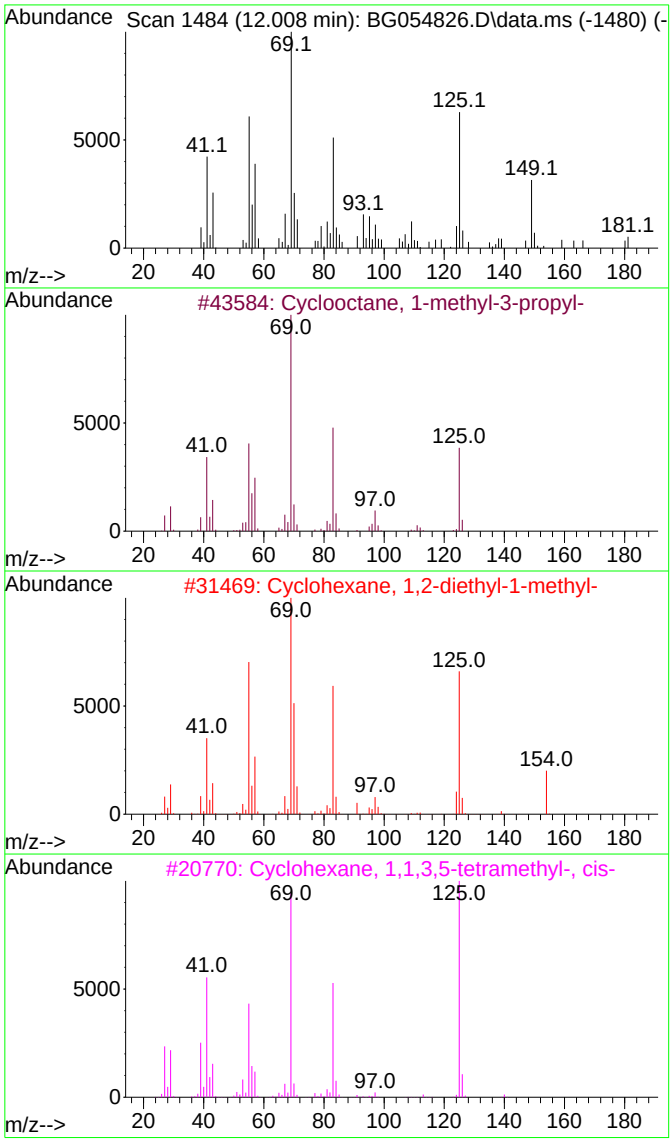
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

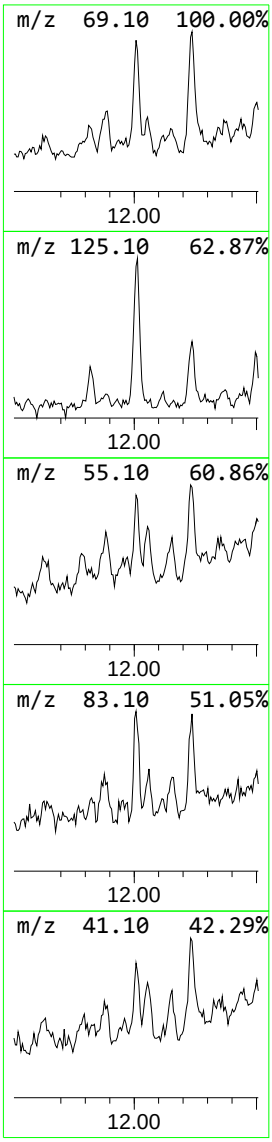
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclooctane, 1-methyl-3-pro... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.008	3.65 ng	64889	Naphthalene-d8	10.973

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclooctane, 1-methyl-3-propyl-	168	C12H24	255885-37-1	59
2	Cyclohexane, 1,2-diethyl-1-methyl-	154	C11H22	061141-79-5	59
3	Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-32-9	50
4	(1,2,4-Trimethylcyclohexyl)metha...	198	C12H22O2	1000499-04-5	47
5	4,4-Dimethyl-non-5-enal	168	C11H20O	066821-98-5	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090122\
Data File : BG054826.D
Acq On : 1 Sep 2022 17:37
Operator : CG/JU
Sample : N4439-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
KTS2-MH-02-0-20

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

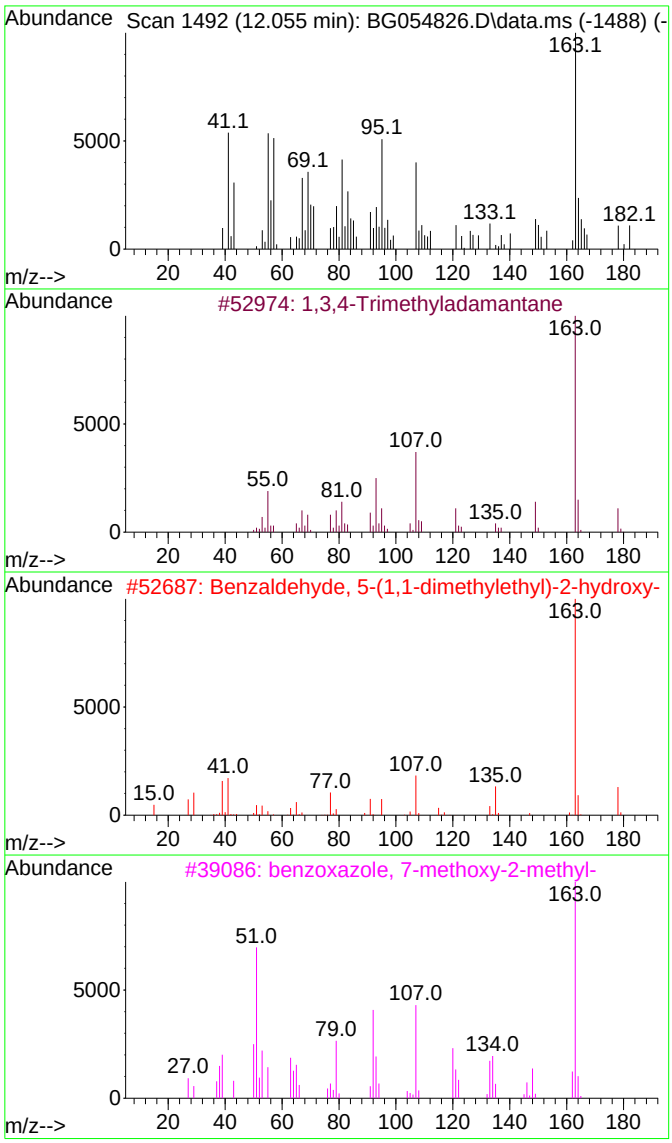
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

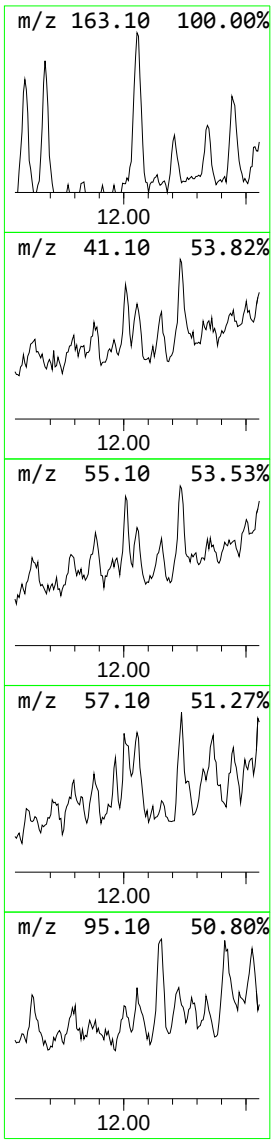
****

Peak Number 4 1,3,4-Trimethyladamantane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.055	4.25 ng	75625	Naphthalene-d8	10.973

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,4-Trimethyladamantane	178	C13H22	1000214-98-3	52
2	Benzaldehyde, 5-(1,1-dimethyleth...	178	C11H14O2	002725-53-3	47
3	benzoxazole, 7-methoxy-2-methyl-	163	C9H9NO2	1000404-43-8	43
4	1,3-Dimethyl-5-ethyladamantane	192	C14H24	001687-35-0	43
5	l-Tyrophanamide	180	C9H12N2O2	1000131-25-3	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090122\
Data File : BG054826.D
Acq On : 1 Sep 2022 17:37
Operator : CG/JU
Sample : N4439-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
KTS2-MH-02-0-20

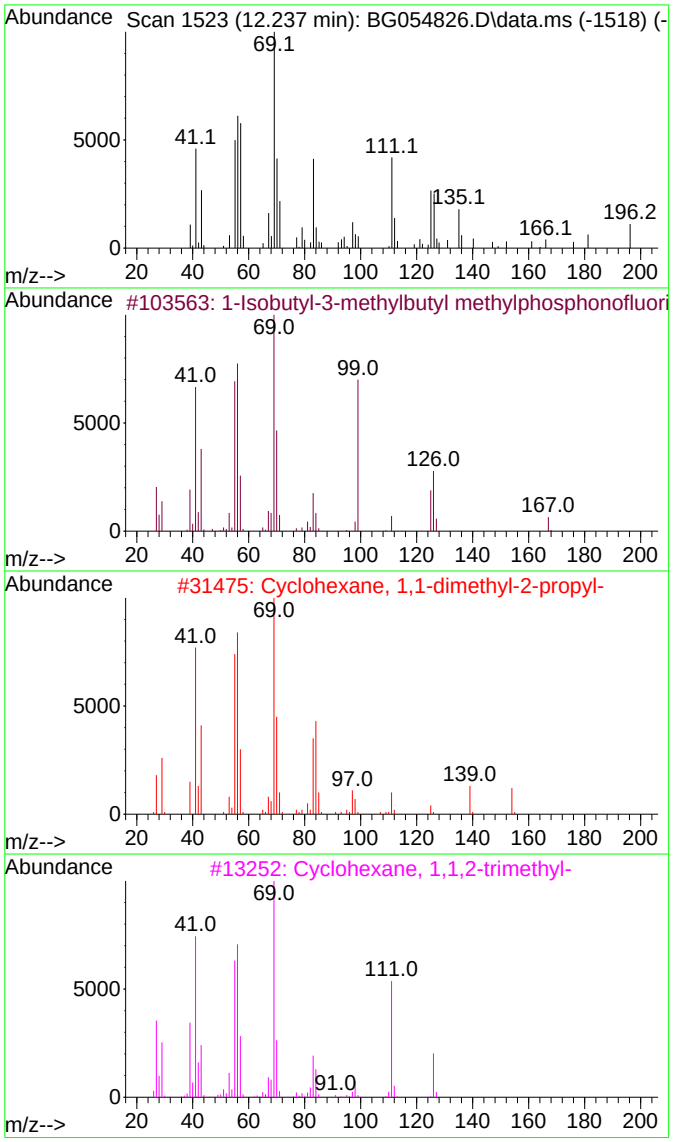
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

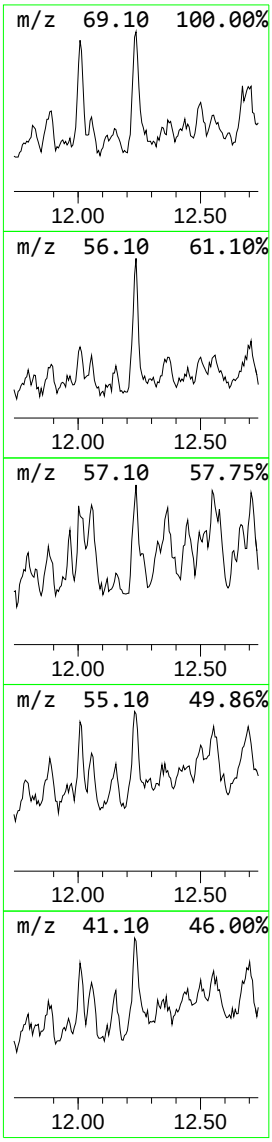
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Isobutyl-3-methylbutyl me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.237	5.55 ng	98700	Naphthalene-d8	10.973

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Isobutyl-3-methylbutyl methylp...	224	C10H22FO2P	193090-16-3	50
2	Cyclohexane, 1,1-dimethyl-2-propyl-	154	C11H22	081983-71-3	50
3	Cyclohexane, 1,1,2-trimethyl-	126	C9H18	007094-26-0	47
4	Cyclooctane, 1-methyl-3-propyl-	168	C12H24	255885-37-1	43
5	4-Decene, 2-methyl-, (E)-	154	C11H22	028665-56-7	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090122\
Data File : BG054826.D
Acq On : 1 Sep 2022 17:37
Operator : CG/JU
Sample : N4439-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
KTS2-MH-02-0-20

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

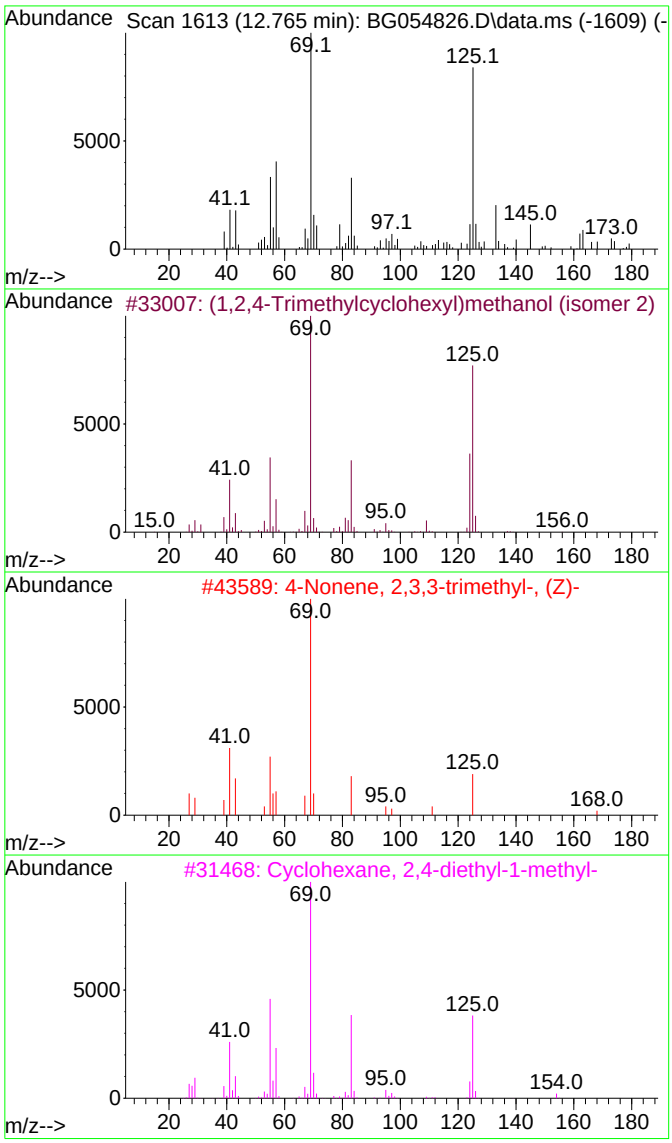
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

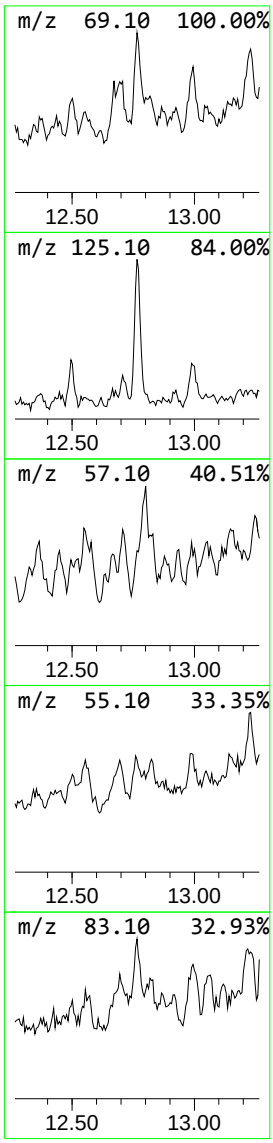
****

Peak Number 6 (1,2,4-Trimethylcyclohexyl)... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.765	3.15 ng	56075	Naphthalene-d8	10.973

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1,2,4-Trimethylcyclohexyl)metha...	156	C10H20O	1000499-03-9	59
2	4-Nonene, 2,3,3-trimethyl-, (Z)-	168	C12H24	063830-68-2	53
3	Cyclohexane, 2,4-diethyl-1-methyl-	154	C11H22	061142-70-9	43
4	(1,2,4-Trimethylcyclohexyl)metha...	198	C12H22O2	1000499-04-5	42
5	(1,2,4-Trimethylcyclohexyl)metha...	156	C10H20O	1000499-04-1	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090122\
Data File : BG054826.D
Acq On : 1 Sep 2022 17:37
Operator : CG/JU
Sample : N4439-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
KTS2-MH-02-0-20

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

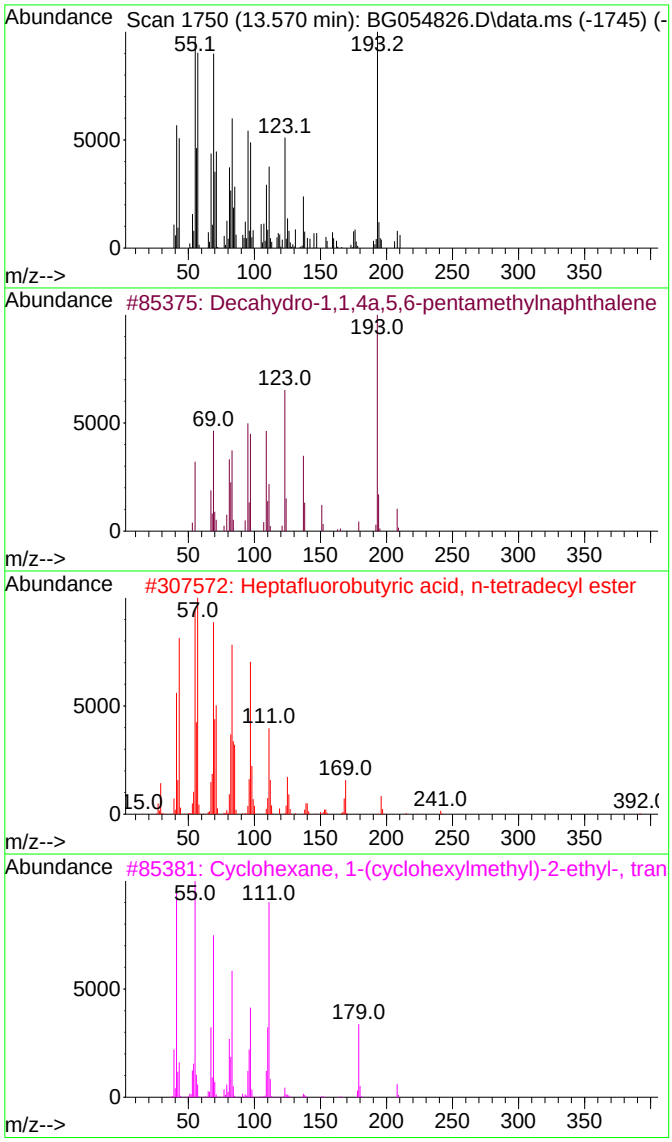
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

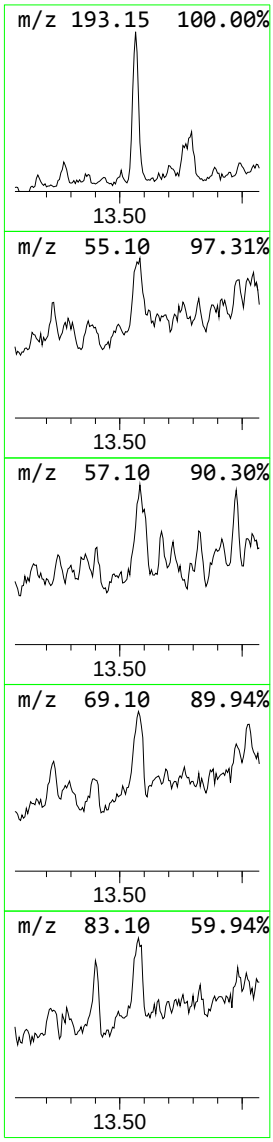
****

Peak Number 7 unknown13.570 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.570	6.39 ng	164587	Acenaphthene-d10	14.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	46
2	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	30
3	Cyclohexane, 1-(cyclohexylmethyl...	208	C15H28	054934-92-8	30
4	3-Methyl-2-(2-oxopropyl)furan	138	C8H10O2	087773-62-4	30
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090122\
Data File : BG054826.D
Acq On : 1 Sep 2022 17:37
Operator : CG/JU
Sample : N4439-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
KTS2-MH-02-0-20

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

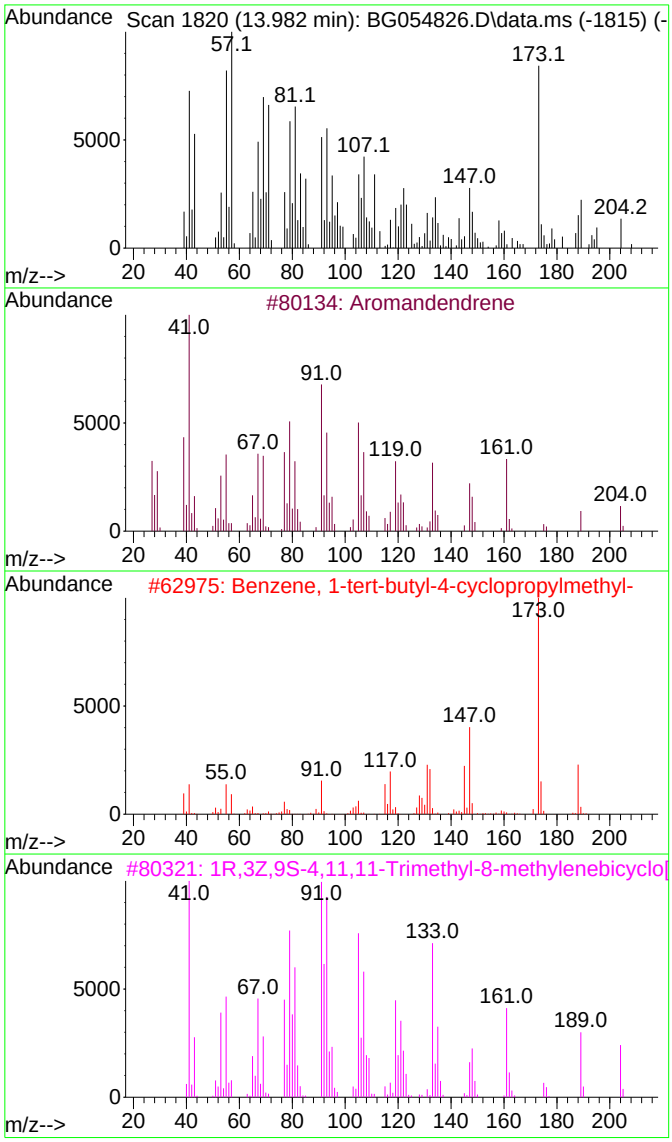
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

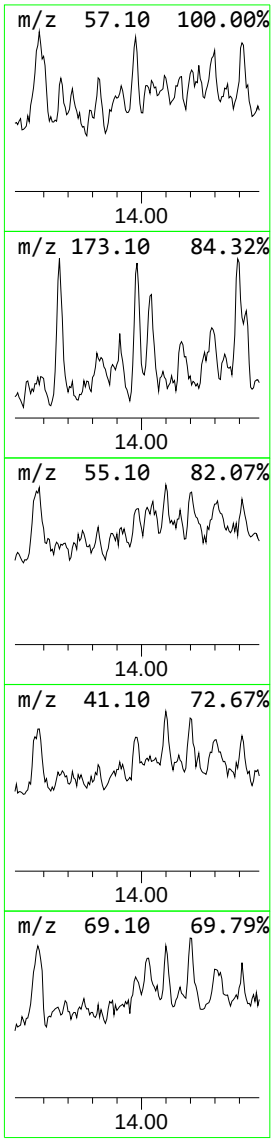
****

Peak Number 8 unknown13.982 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.982	5.21 ng	134045	Acenaphthene-d10	14.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aromandendrene	204	C15H24	000489-39-4	42
2	Benzene, 1-tert-butyl-4-cyclopro...	188	C14H20	058249-45-9	38
3	1R,3Z,9S-4,11,11-Trimethyl-8-met...	204	C15H24	1000159-39-4	35
4	1H-1,5-Benzodiazepine, 2,3-dihyd...	188	C12H16N2	024107-34-4	30
5	Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	25





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Acq On : 1 Sep 2022 17:37
Operator : CG/JU
Sample : N4439-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

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ClientSampleId :
KTS2-MH-02-0-20

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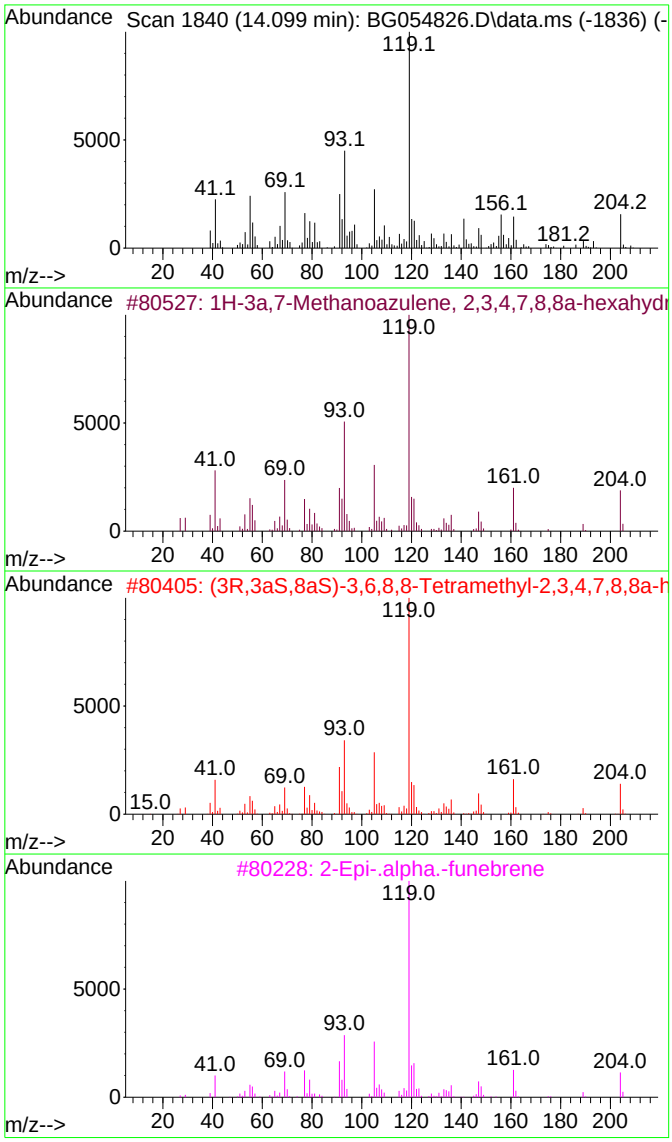
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

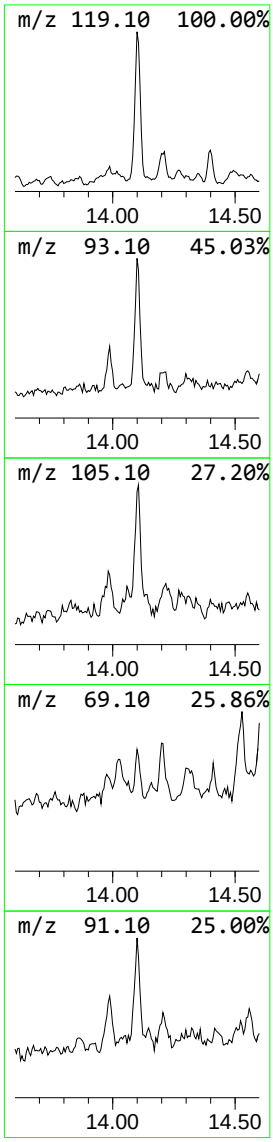
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1H-3a,7-Methanoazulene, 2,3... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.099	5.91 ng	152216	Acenaphthene-d10	14.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-3a,7-Methanoazulene, 2,3,4,7,...	204	C15H24	000469-61-4	98
2	(3R,3aS,8aS)-3,6,8,8-Tetramethyl...	204	C15H24	022567-43-7	98
3	2-Epi-.alpha.-funebrene	204	C15H24	065354-33-8	95
4	Di-epi-.alpha.-cedrene	204	C15H24	050894-66-1	87
5	trans-.alpha.-Bergamotene	204	C15H24	013474-59-4	76





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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

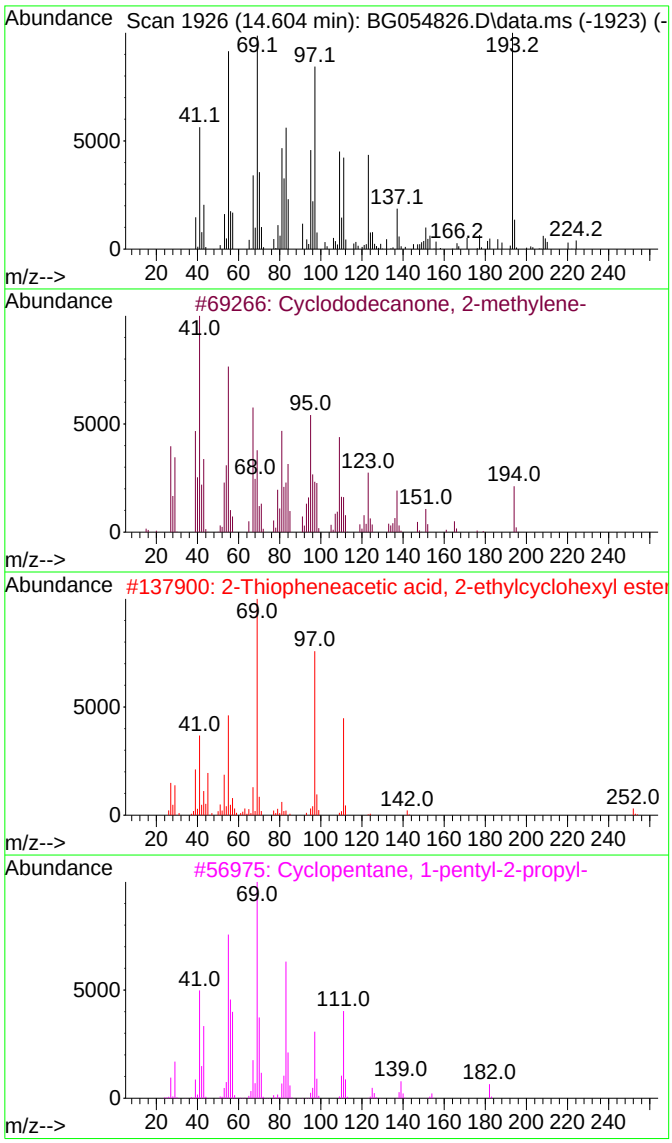
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

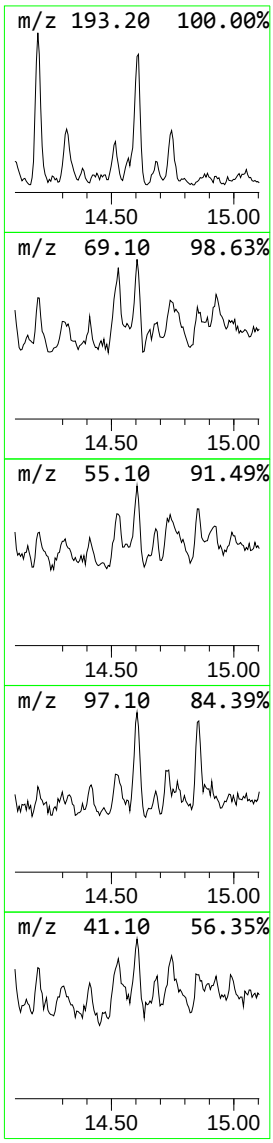
****

Peak Number 10 unknown14.605 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.605	5.93 ng	152605	Acenaphthene-d10	14.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	38
2	2-Thiopheneacetic acid, 2-ethylc...	252	C14H20O2S	1000278-96-1	35
3	Cyclopentane, 1-pentyl-2-propyl-	182	C13H26	062199-51-3	30
4	Hexahydro-1-oxa-cyclopropa[d]ind...	152	C9H12O2	037643-23-5	27
5	4-Hexen-3-one, 4,5-dimethyl-	126	C8H14O	017325-90-5	22





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ClientSampleId :
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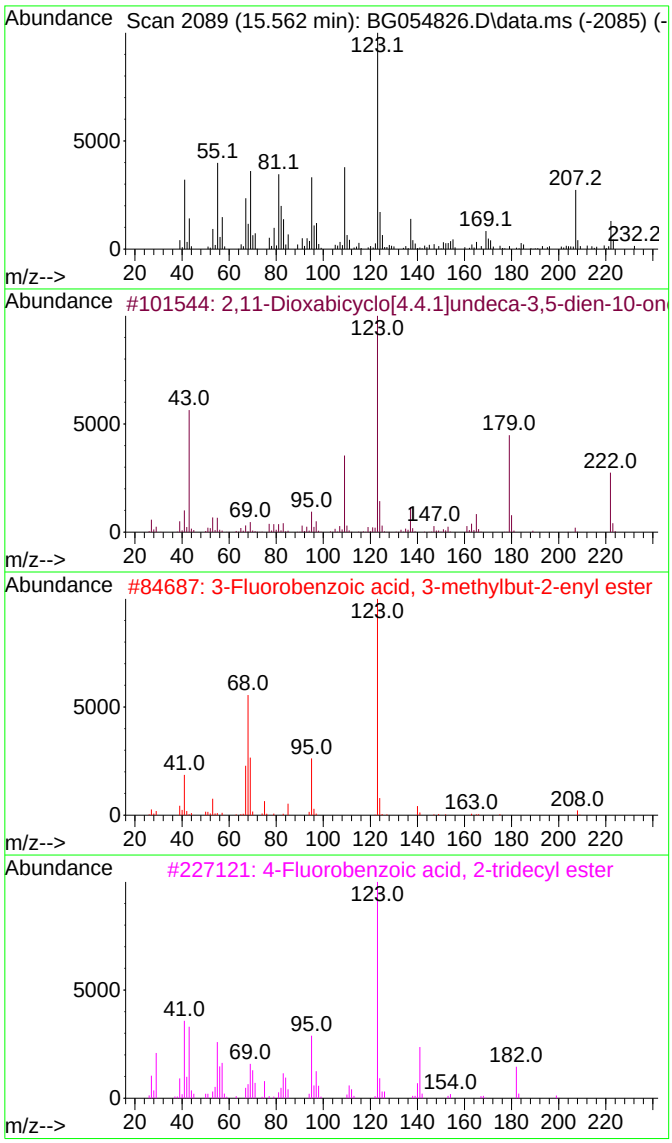
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

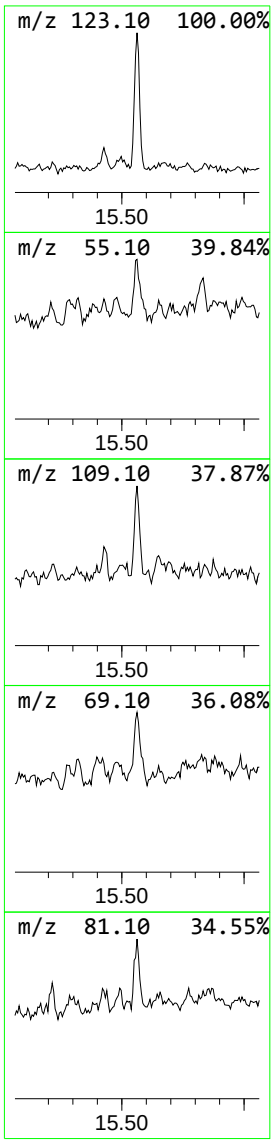
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 2,11-Dioxabicyclo[4.4.1]und... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.562	6.39 ng	164596	Acenaphthene-d10	14.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,11-Dioxabicyclo[4.4.1]undeca-3...	222	C13H18O3	070412-52-1	53
2	3-Fluorobenzoic acid, 3-methylbu...	208	C12H13FO2	154559-38-3	49
3	4-Fluorobenzoic acid, 2-tridecyl...	322	C20H31FO2	1000280-67-8	47
4	photocitral A	152	C10H16O	055253-28-6	47
5	4-Fluorobenzoic acid, 1-cyclopen...	236	C14H17FO2	1000279-05-8	47





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BNA_G
ClientSampleId :
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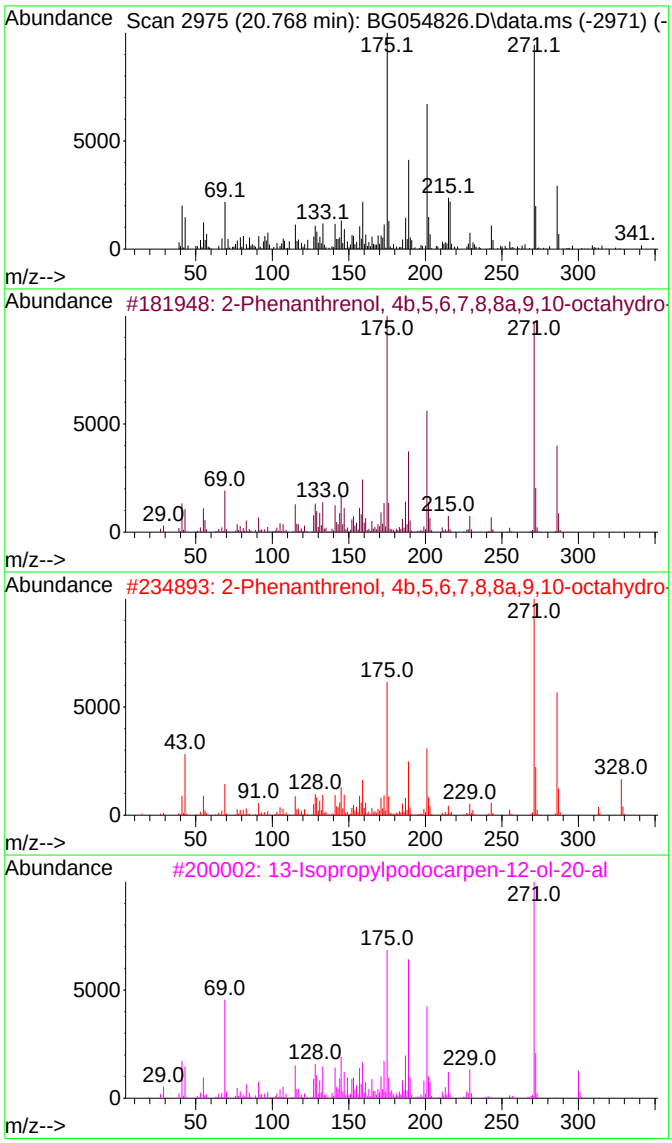
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

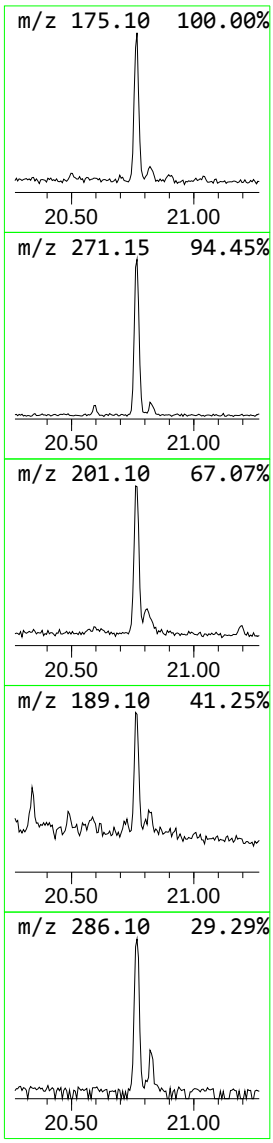
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.768	5.04 ng	155697	Chrysene-d12	21.820

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	99
2	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	328	C22H32O2	015340-82-6	83
3	13-Isopropylpodocarpen-12-ol-20-al	300	C20H28O2	024035-37-8	35
4	Propionic acid, 3,3,3-trifluoro-...	330	C15H13F3O3S	1000276-91-1	27
5	Oxazole, 2-(1-naphthalenyl)-5-ph...	271	C19H13NO	000846-63-9	22





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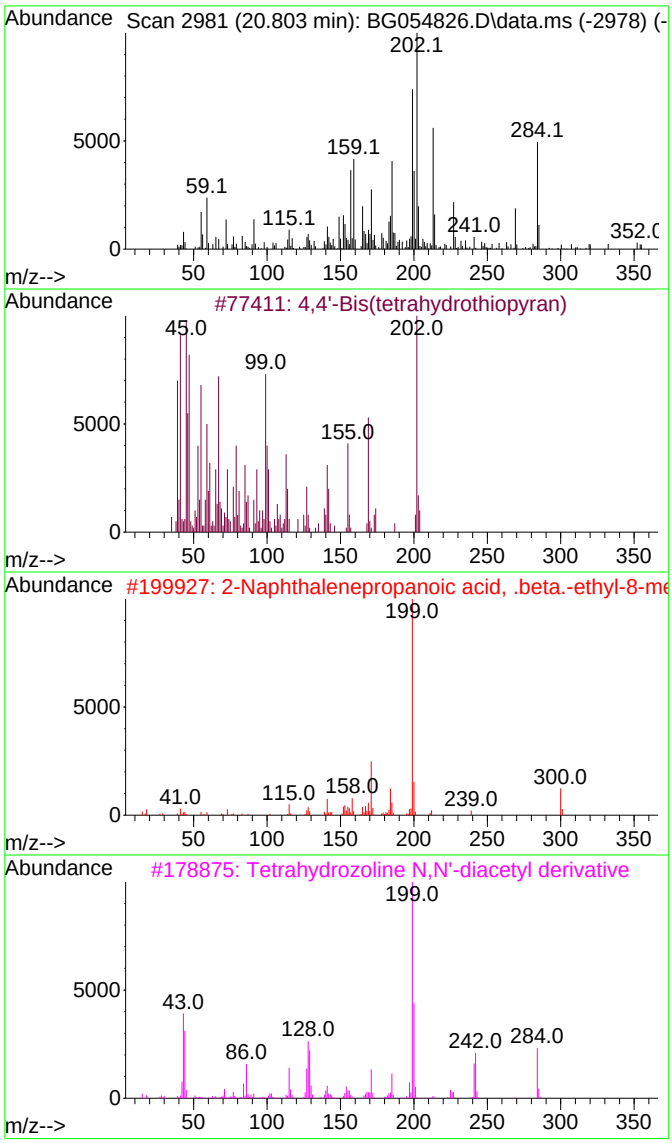
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

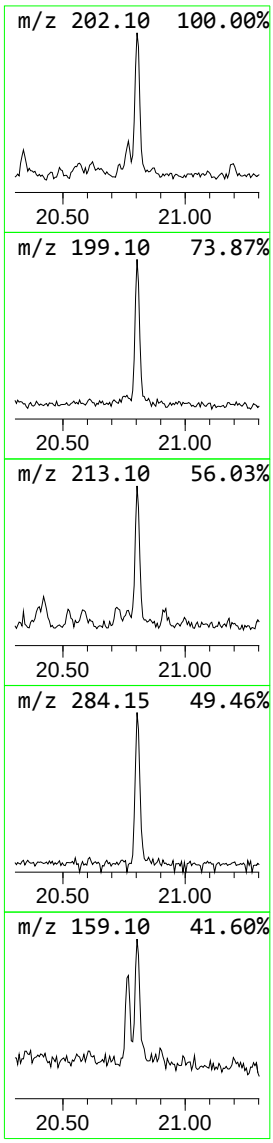
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 4,4'-Bis(tetrahydrothiopyran) Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.803	5.37 ng	165815	Chrysene-d12	21.820

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	56
2	2-Naphthalenepropanoic acid, .be...	300	C19H24O3	057289-69-7	25
3	Tetrahydrozoline N,N'-diacetyl d...	284	C17H20N2O2	1010442-80-7	22
4	[1,2,5]-Oxadiazolo[3,4-a]cinnoli...	202	C10H10N4O	1000260-59-4	18
5	2-Benzyl-6-methyl-4(3H)-pyrimidi...	200	C12H12N2O	016673-85-1	15





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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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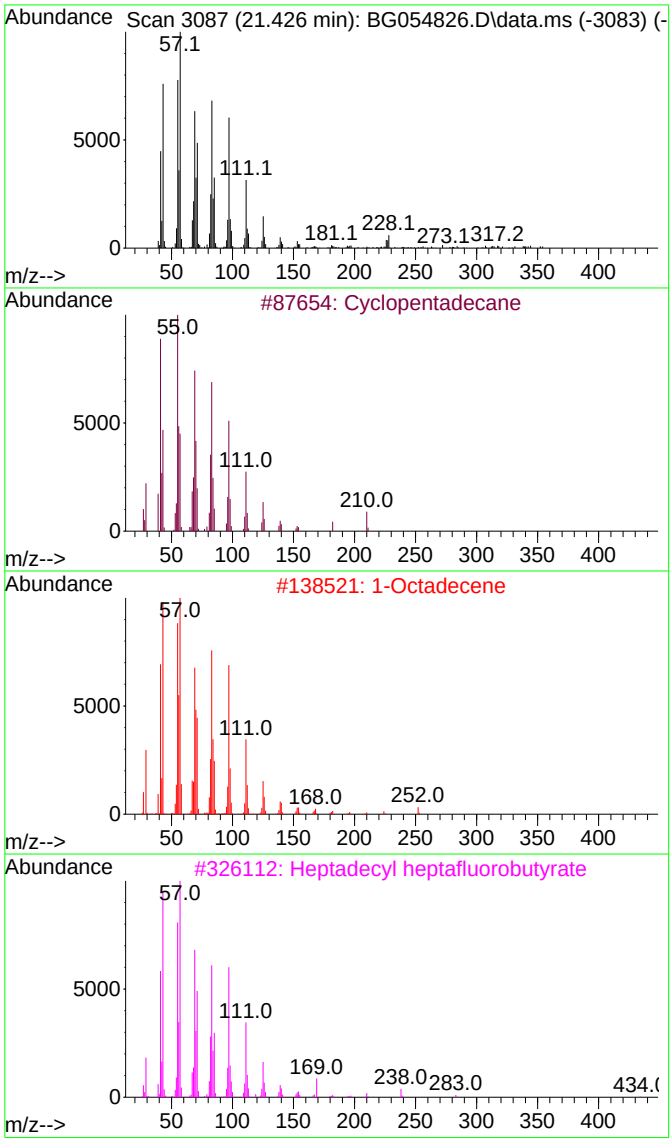
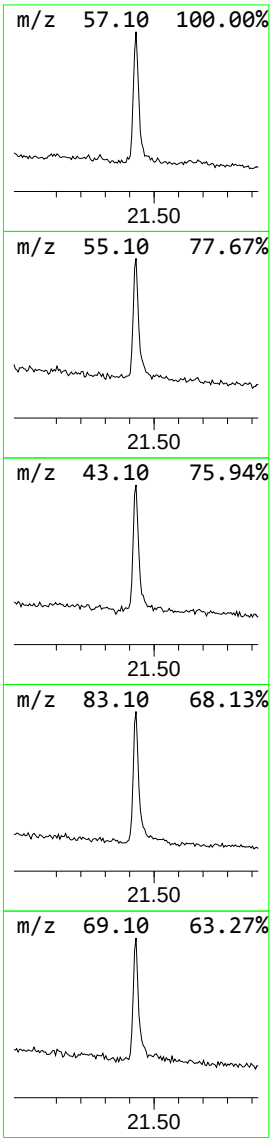
Peak Number 14 Cyclopentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.426	11.58 ng	357676	Chrysene-d12	21.820

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	96
2	1-Octadecene	252	C18H36	000112-88-9	95
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
5	1-Hexacosene	364	C26H52	018835-33-1	94





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Sample : N4439-03
Misc :
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Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

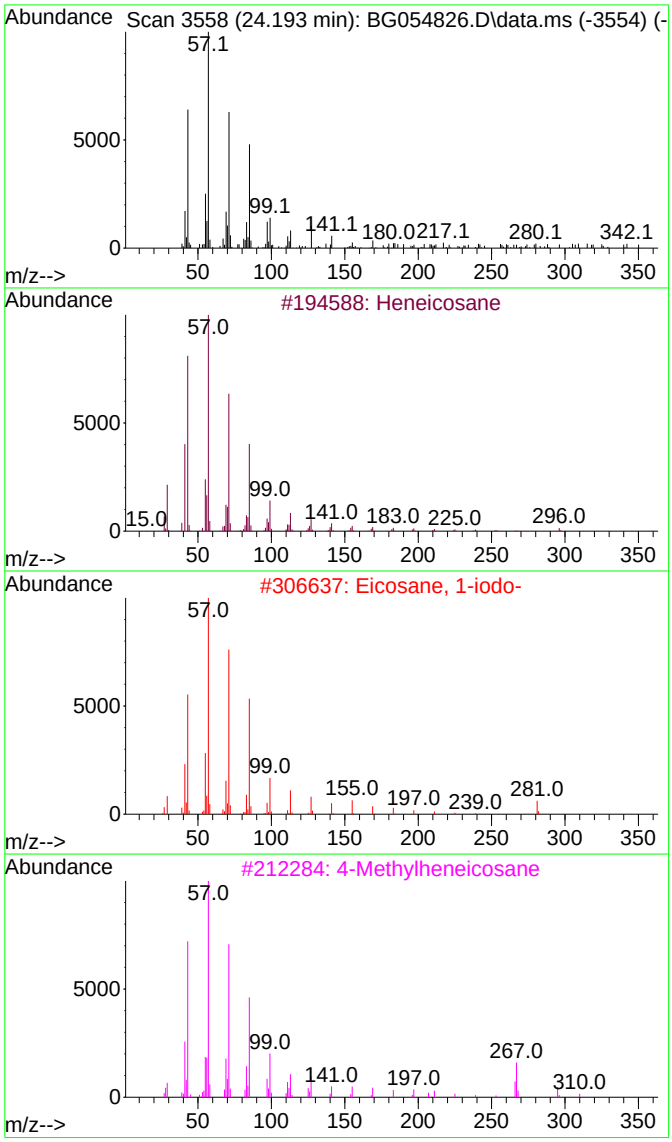
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

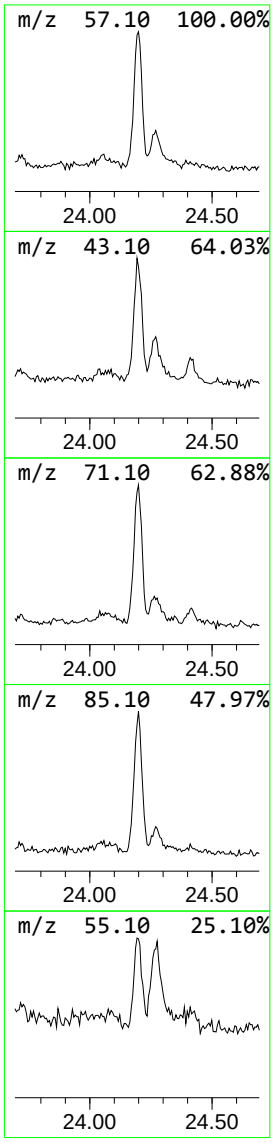
****

Peak Number 15 Heneicosane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.193	4.03 ng	137432	Perylene-d12	25.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	92
2	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	87
3	4-Methylheneicosane	310	C22H46	025117-29-7	87
4	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	87
5	Tetracosane	338	C24H50	000646-31-1	87





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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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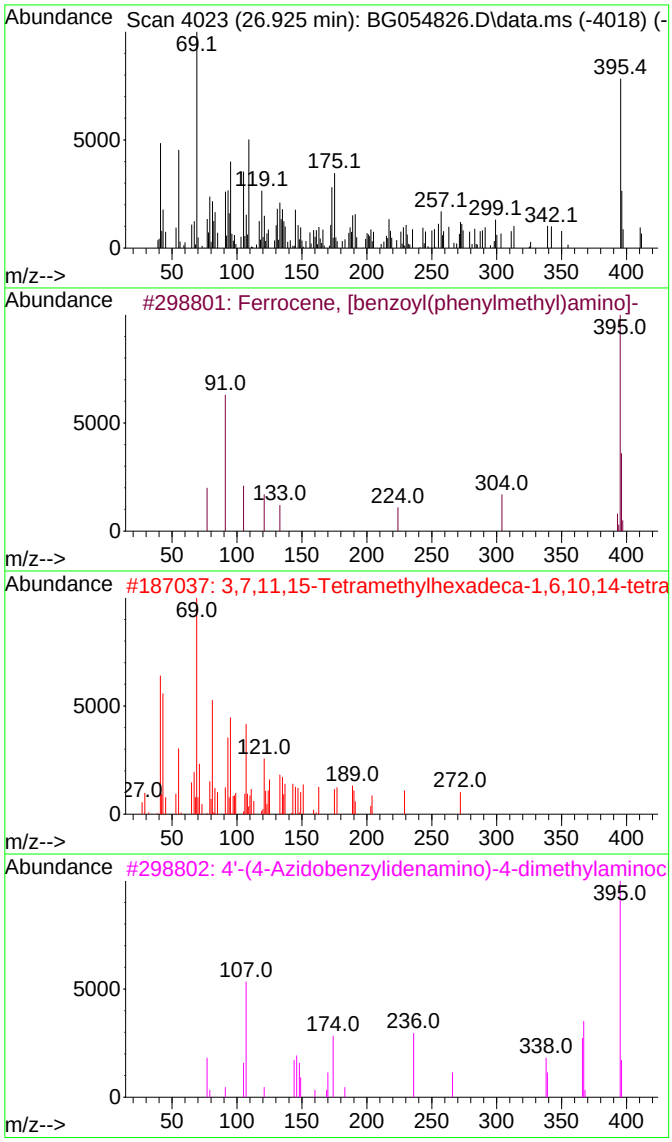
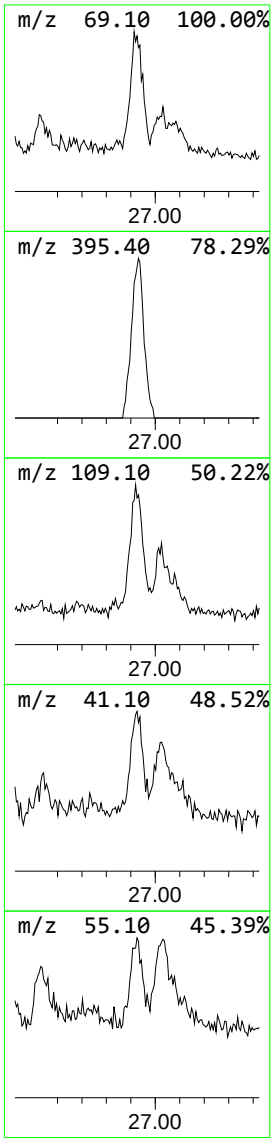
Peak Number 16 unknown26.925 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.925	3.78 ng	128658	Perylene-d12	25.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ferrocene, [benzoyl(phenylmethyl...	395	C24H21FeNO	012156-49-9	35
2	3,7,11,15-Tetramethylhexadeca-1,...	290	C20H34O	068931-30-6	27
3	4'-(4-Azidobenzylidenamino)-4-di...	395	C24H21N5O	1000110-92-4	17
4	1-(2-Naphthyloxy)-4-nitroanthraq...	395	C24H13NO5	1000110-92-3	14
5	Benzonitrile, 4-(4'-ethyl[1,1'-b...	313	C21H28FN	100822-13-7	14





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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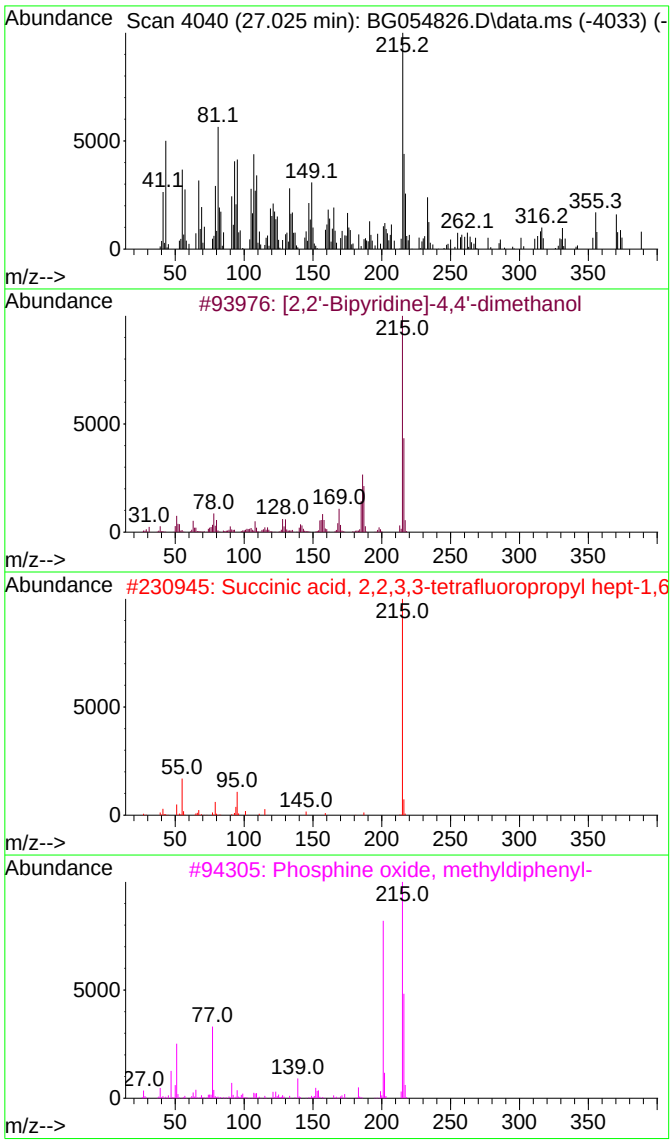
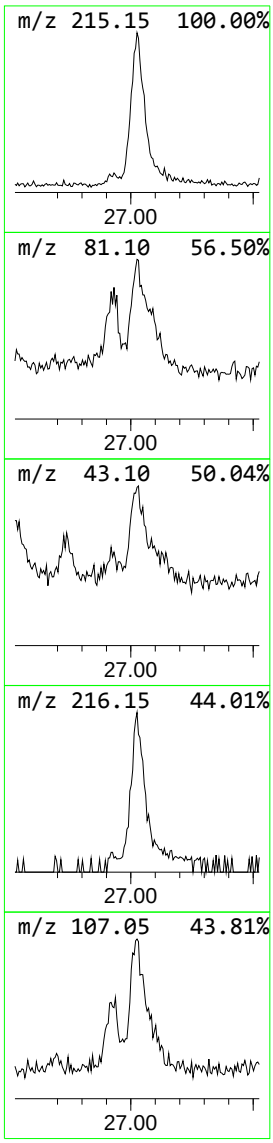
Peak Number 17 unknown27.025 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.025	7.69 ng	262099	Perylene-d12	25.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	[2,2'-Bipyridine]-4,4'-dimethanol	216	C12H12N2O2	109073-77-0	38
2	Succinic acid, 2,2,3,3-tetrafluo...	326	C14H18F4O4	1000391-32-6	35
3	Phosphine oxide, methyldiphenyl-	216	C13H13OP	002129-89-7	35
4	CP 47,497 (n=7)	318	C21H34O2	070434-82-1	35
5	Cyclopent[e]-1,3-oxazine, octahy...	216	C13H16N2O	1000138-92-2	35





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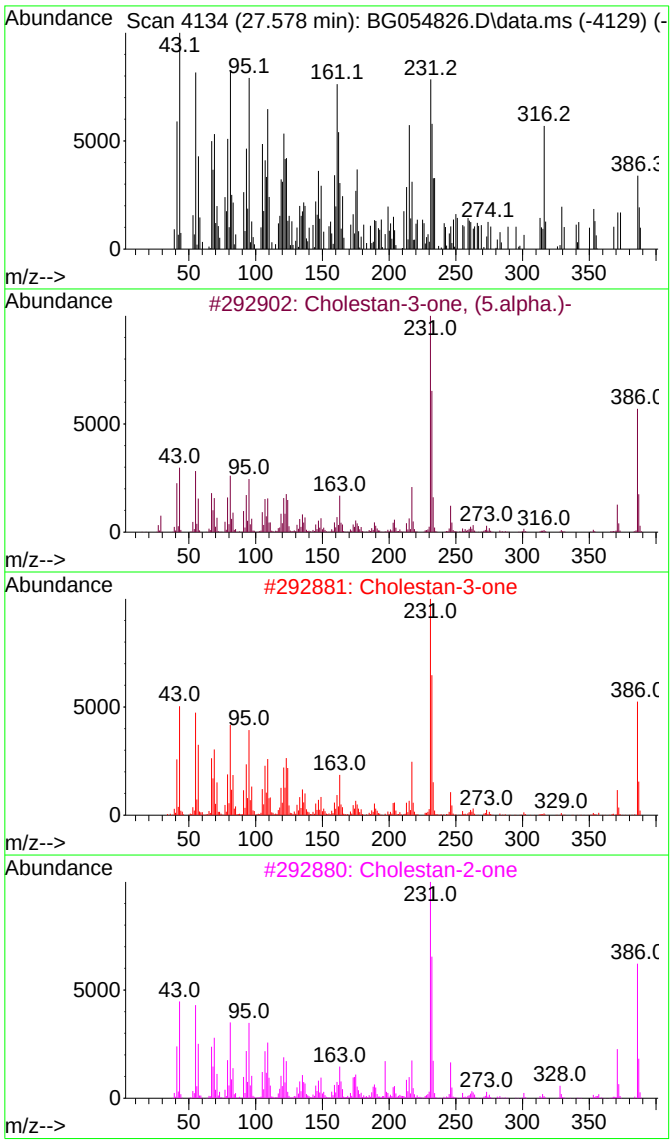
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

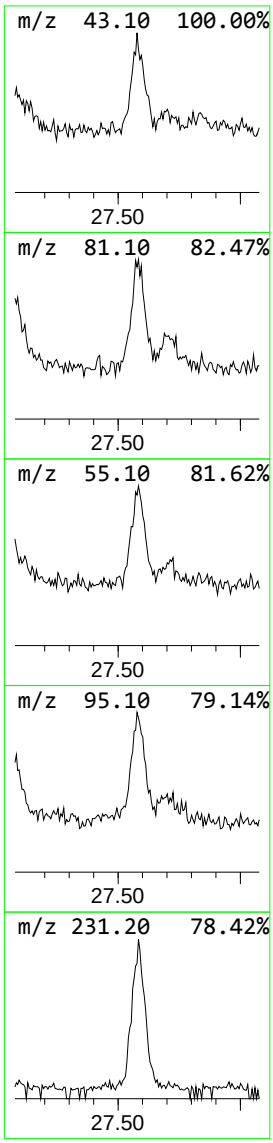
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 Cholestan-3-one, (5.alpha.)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.578	7.34 ng	249977	Perylene-d12	25.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholestan-3-one, (5.alpha.)-	386	C27H46O	000566-88-1	70
2	Cholestan-3-one	386	C27H46O	015600-08-5	55
3	Cholestan-2-one	386	C27H46O	1010210-43-4	49
4	Cholest-2-en-1-ol	386	C27H46O	1000210-36-4	41
5	1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	017334-55-3	25





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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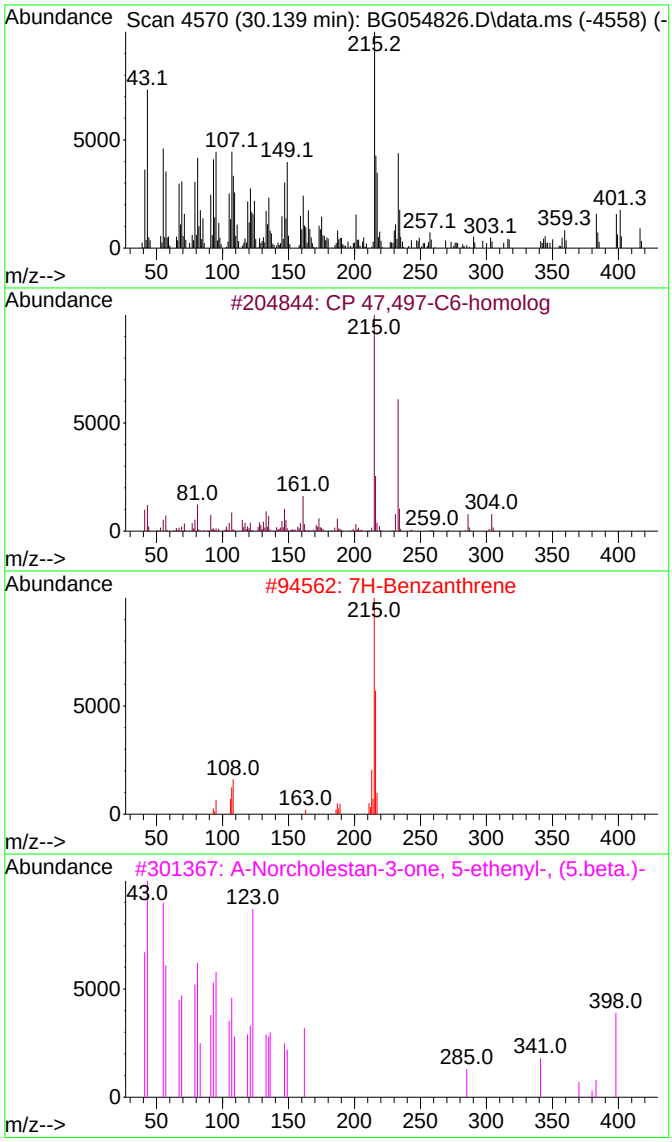
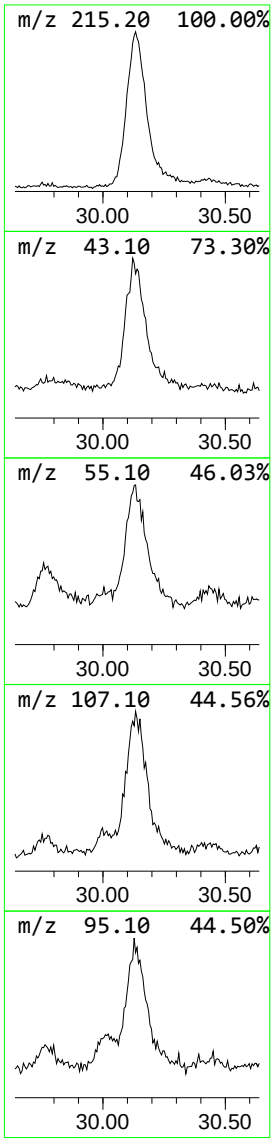
Peak Number 19 unknown30.139 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.139	25.23 ng	859769	Perylene-d12	25.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	CP 47,497-C6-homolog	304	C20H32O2	070435-06-2	35
2	7H-Benzanthrene	216	C17H12	000199-94-0	27
3	A-Norcholestan-3-one, 5-ethenyl-...	398	C28H46O	019594-90-2	25
4	5-(2-Methyloctan-2-yl)-3-(1R,3R-...	332	C22H36O2	070434-92-3	22
5	CP 47,497 (n=7)	318	C21H34O2	070434-82-1	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090122\
Data File : BG054826.D
Acq On : 1 Sep 2022 17:37
Operator : CG/JU
Sample : N4439-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
KTS2-MH-02-0-20

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

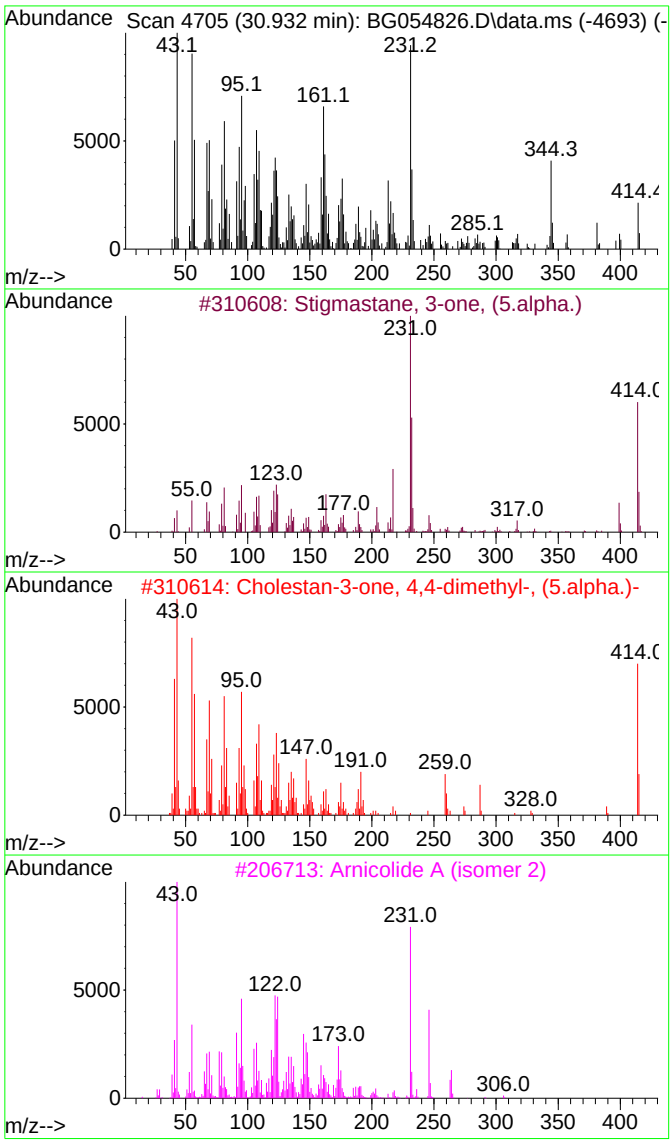
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

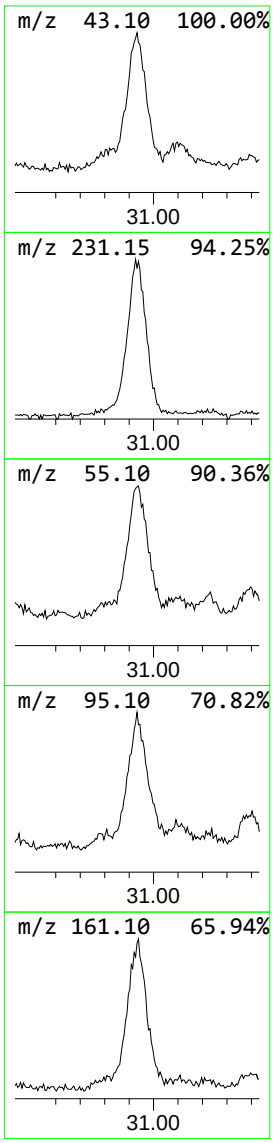
****

Peak Number 20 unknown30.932 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.932	30.47 ng	1038480	Perylene-d12	25.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Stigmastane, 3-one, (5.alpha.)	414	C29H50O	1000437-00-8	41
2	Cholestan-3-one, 4,4-dimethyl-, ...	414	C29H50O	002097-85-0	35
3	Arnicolide A (isomer 2)	306	C17H22O5	1000495-69-8	35
4	Cyclohexanol, 3-ethenyl-3-methyl...	222	C15H26O	035727-45-8	25
5	3-(3,5-Dimethylpyrazol-1-yl)-4-(...	246	C10H10N6O2	1000436-49-9	18





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090122\
Data File : BG054826.D
Acq On : 1 Sep 2022 17:37
Operator : CG/JU
Sample : N4439-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
KTS2-MH-02-0-20

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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-...	5.210	6.6	ng	79055	1	8.147	238972	20.0
4-Nonene, 5-butyl-	11.449	3.6	ng	64884	2	10.973	355821	20.0
Cyclooctane, 1-...	12.008	3.6	ng	64889	2	10.973	355821	20.0
1,3,4-Trimethyl...	12.055	4.3	ng	75625	2	10.973	355821	20.0
1-Isobutyl-3-me...	12.237	5.5	ng	98700	2	10.973	355821	20.0
(1,2,4-Trimethy...	12.765	3.1	ng	56075	2	10.973	355821	20.0
unknown13.570	13.570	6.4	ng	164587	3	14.781	514962	20.0
unknown13.982	13.982	5.2	ng	134045	3	14.781	514962	20.0
1H-3a,7-Methano...	14.099	5.9	ng	152216	3	14.781	514962	20.0
unknown14.605	14.605	5.9	ng	152605	3	14.781	514962	20.0
2,11-Dioxabicyc...	15.562	6.4	ng	164596	3	14.781	514962	20.0
2-Phenanthrenol...	20.768	5.0	ng	155697	5	21.820	617536	20.0
4,4'-Bis(tetrah...	20.803	5.4	ng	165815	5	21.820	617536	20.0
Cyclopentadecane	21.426	11.6	ng	357676	5	21.820	617536	20.0
Heneicosane	24.193	4.0	ng	137432	6	25.186	681552	20.0
unknown26.925	26.925	3.8	ng	128658	6	25.186	681552	20.0
unknown27.025	27.025	7.7	ng	262099	6	25.186	681552	20.0
Cholestan-3-one...	27.578	7.3	ng	249977	6	25.186	681552	20.0
unknown30.139	30.139	25.2	ng	859769	6	25.186	681552	20.0
unknown30.932	30.932	30.5	ng	1038480	6	25.186	681552	20.0