LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052523\
Data File : BF133492.D
Acq On : 25 May 2023 16:16
Operator : CG\JU
Sample : PB153012BL
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB153012BL

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-BF052523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133492.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.157	4	12	18	rVB	94433	131286	2.23%	0.339%
2	4.434	395	399	405	rVB	335447	391398	6.64%	1.012%
3	5.063	500	506	516	rBV	979585	1464907	24.86%	3.787%
4	5.457	567	573	576	rBV	3902524	4675556	79.33%	12.087%
5	5.851	637	640	644	rVB	106178	84676	1.44%	0.219%
6	6.463	737	744	747	rBV	3475903	4785163	81.19%	12.370%
7	6.834	804	807	811	rVB	1139346	990900	16.81%	2.562%
8	7.404	897	904	907	rBV	2919208	3073985	52.16%	7.947%
9	8.122	1021	1026	1029	rBV	1552487	1323040	22.45%	3.420%
10	9.204	1203	1210	1213	rBV	5223915	5188358	88.03%	13.412%
11	9.875	1320	1324	1328	rBV	1817135	1460396	24.78%	3.775%
12	10.669	1454	1459	1462	rBV	3559174	3522290	59.76%	9.105%
13	11.363	1573	1577	1580	rBV	1996712	1613599	27.38%	4.171%
14	12.963	1843	1849	1852	rBV	5309057	5893798	100.00%	15.236%
15	14.004	2022	2026	2029	rBV	1645414	1415714	24.02%	3.660%
16	14.792	2156	2160	2163	rBV	70567	68441	1.16%	0.177%
17	15.133	2213	2218	2224	rBV	92971	105398	1.79%	0.272%
18	15.462	2268	2274	2279	rBV	1158495	1418890	24.07%	3.668%
19	15.515	2279	2283	2289	rVB	123171	160637	2.73%	0.415%
20	15.951	2352	2357	2364	rBV	98742	151675	2.57%	0.392%
21	16.462	2438	2444	2455	rBV	85287	156368	2.65%	0.404%
22	16.980	2515	2532	2542	rBV4	73694	419540	7.12%	1.085%
23	17.056	2542	2545	2555	rVB2	56901	114202	1.94%	0.295%
24	17.768	2660	2666	2678	rVB4	28496	73242	1.24%	0.189%

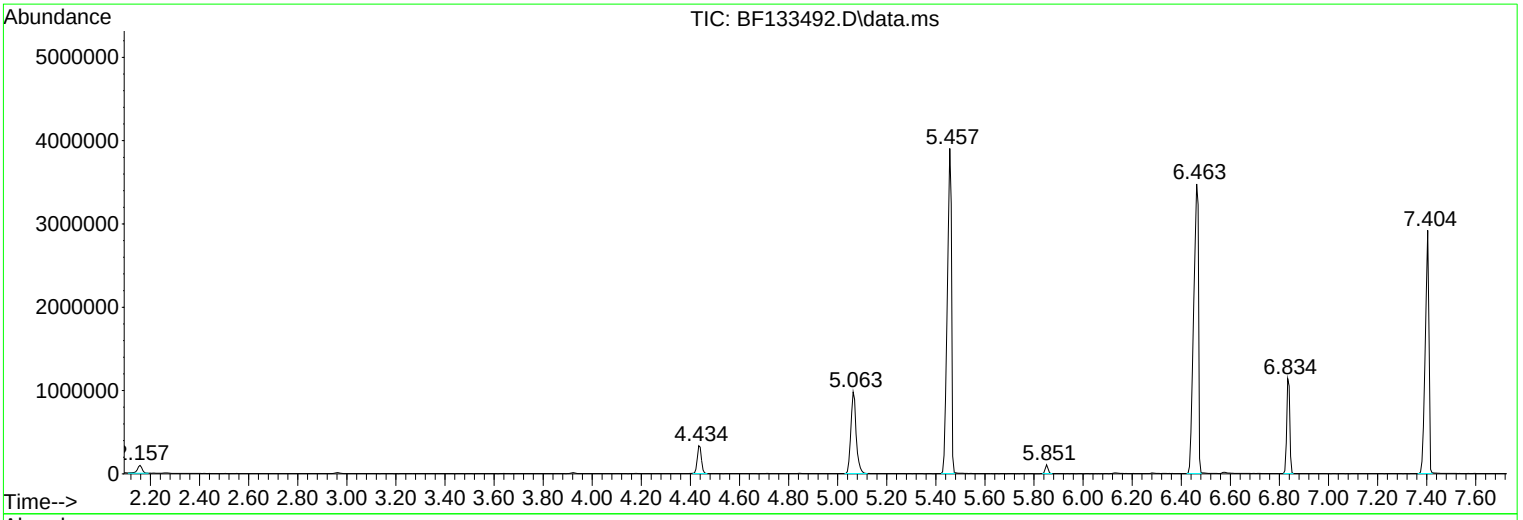
Sum of corrected areas: 38683459

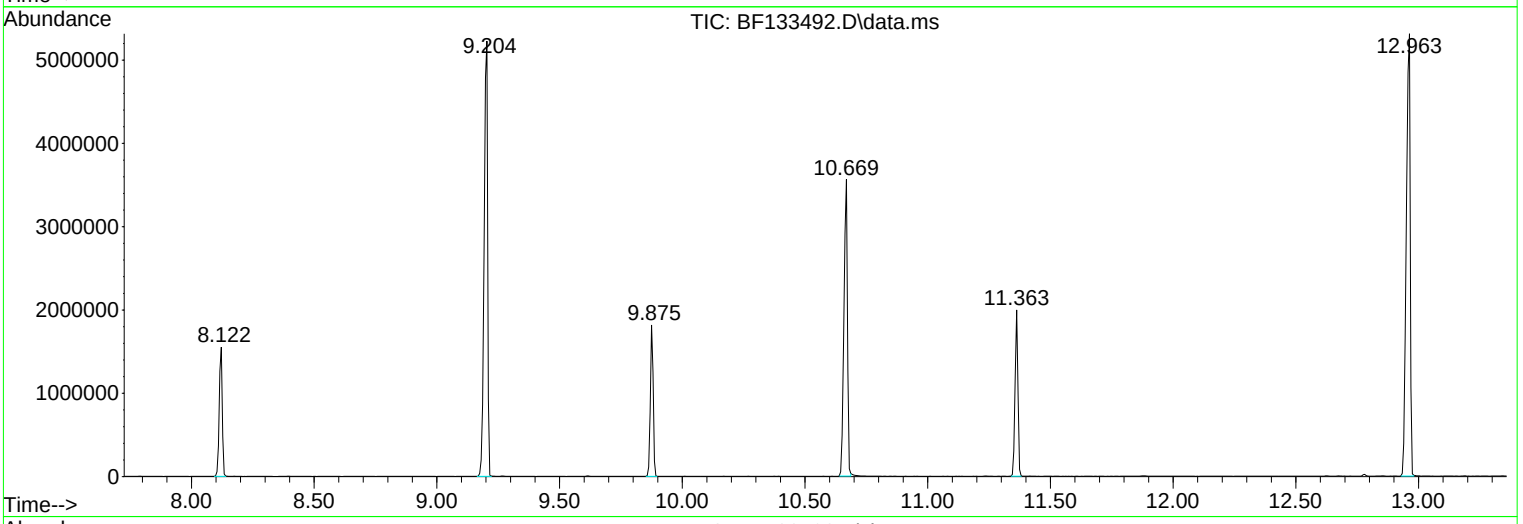
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052523\
Data File : BF133492.D
Acq On : 25 May 2023 16:16
Operator : CG\JU
Sample : PB153012BL
Misc :
ALS Vial : 11 Sample Multiplier: 1

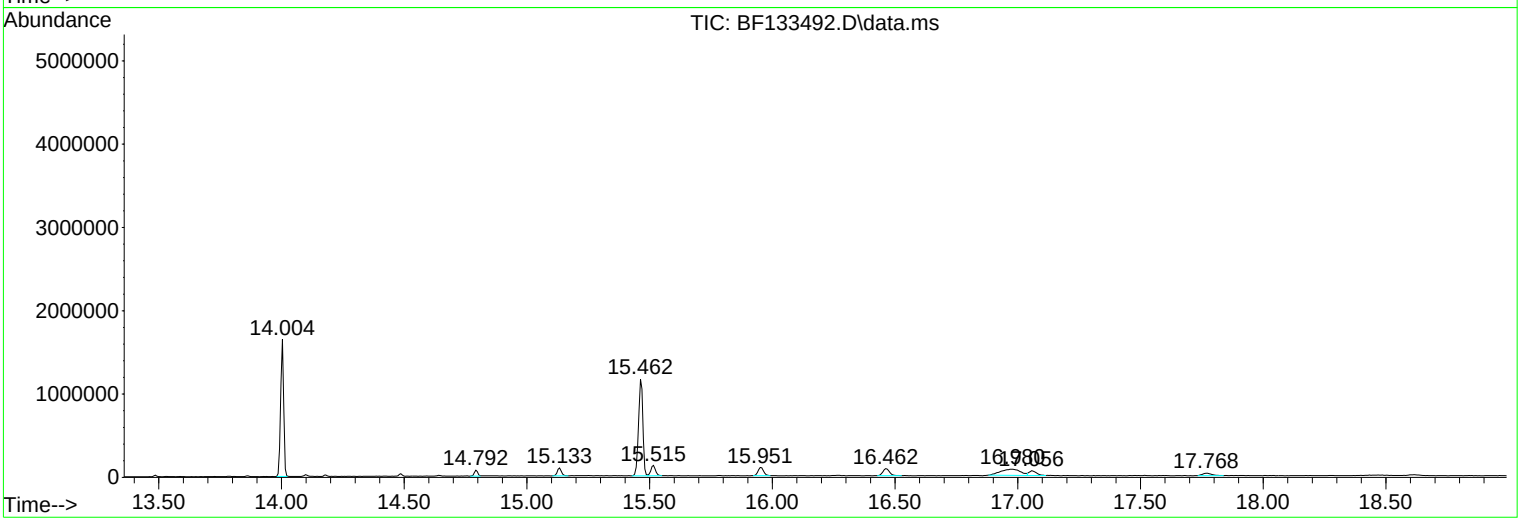
Instrument :
BNA_F
ClientSampleId :
PB153012BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.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\BF052523\
Data File : BF133492.D
Acq On : 25 May 2023 16:16
Operator : CG\JU
Sample : PB153012BL
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB153012BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

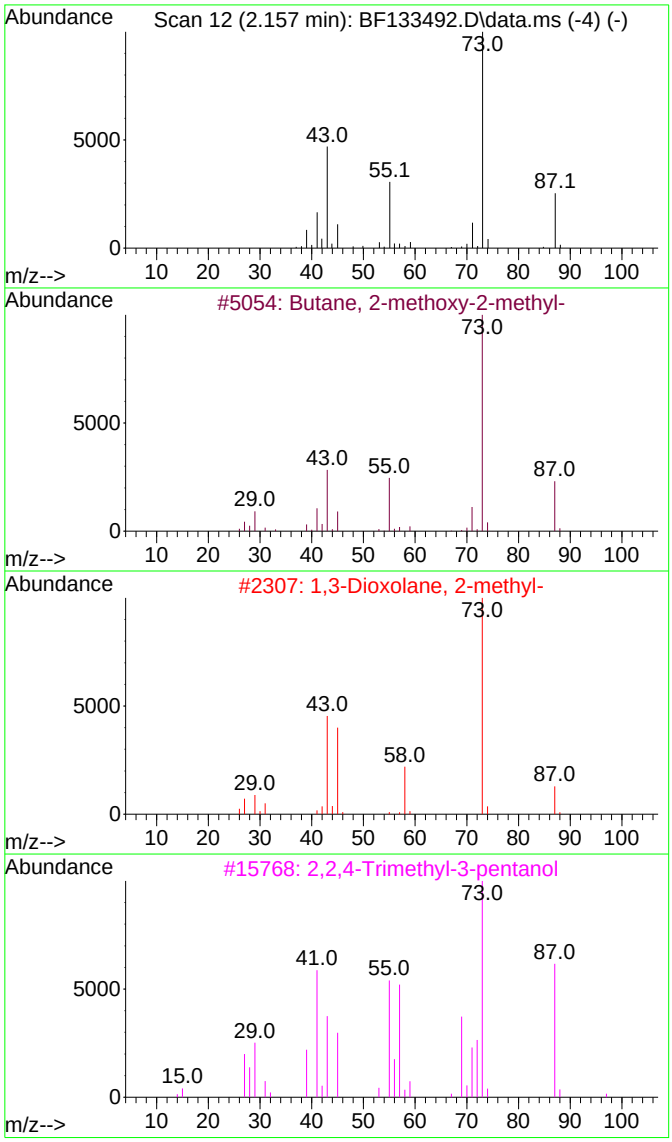
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

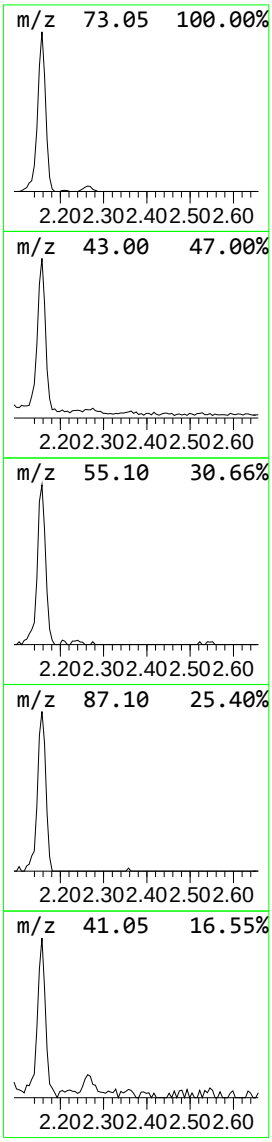
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.157	2.65 ng	131286	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	47
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052523\
Data File : BF133492.D
Acq On : 25 May 2023 16:16
Operator : CG\JU
Sample : PB153012BL
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB153012BL

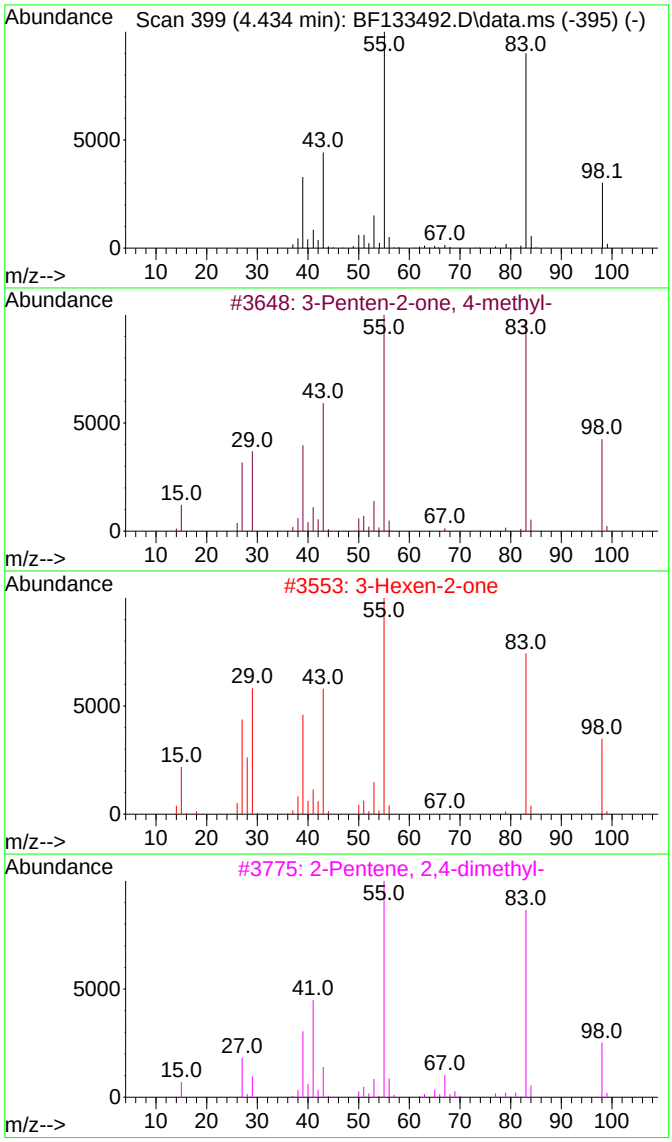
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

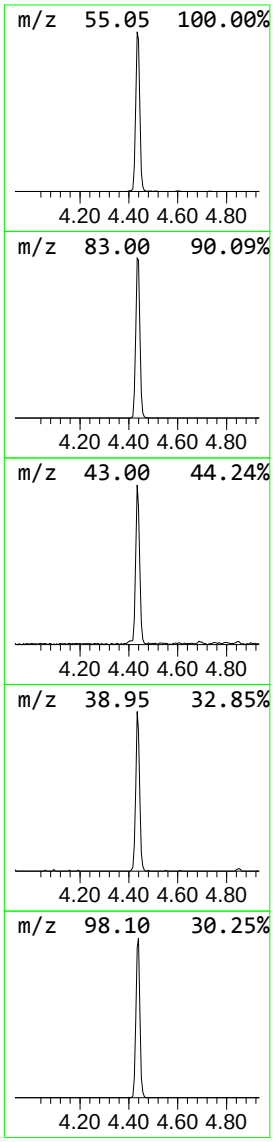
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.434	7.90 ng	391398	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
4	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
5	2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052523\
Data File : BF133492.D
Acq On : 25 May 2023 16:16
Operator : CG\JU
Sample : PB153012BL
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB153012BL

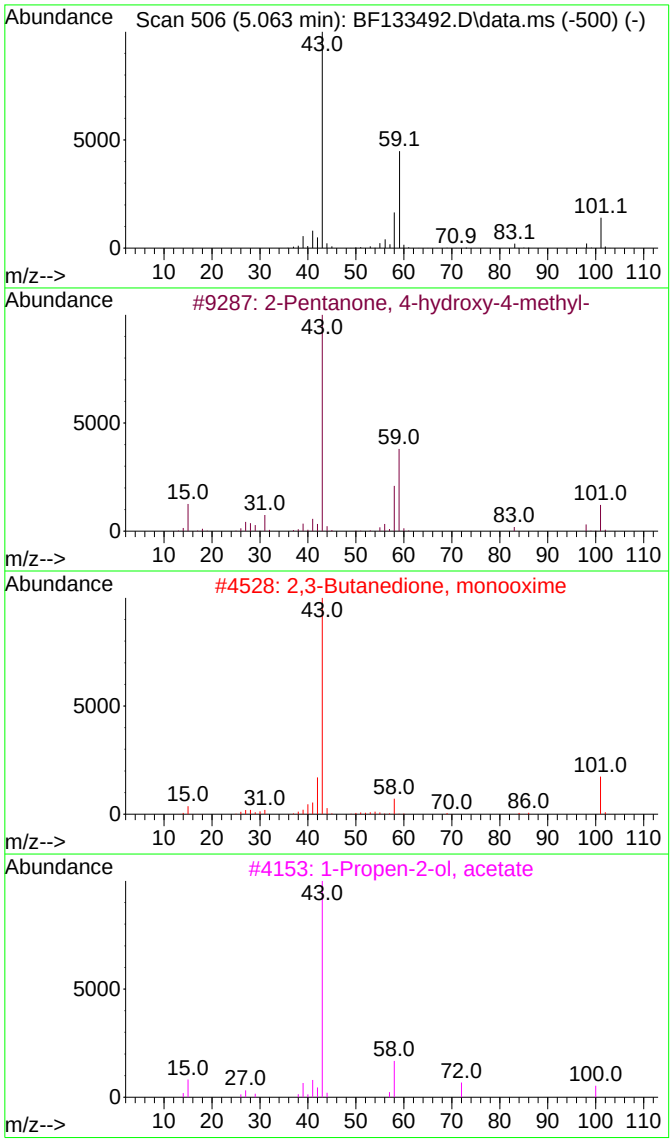
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

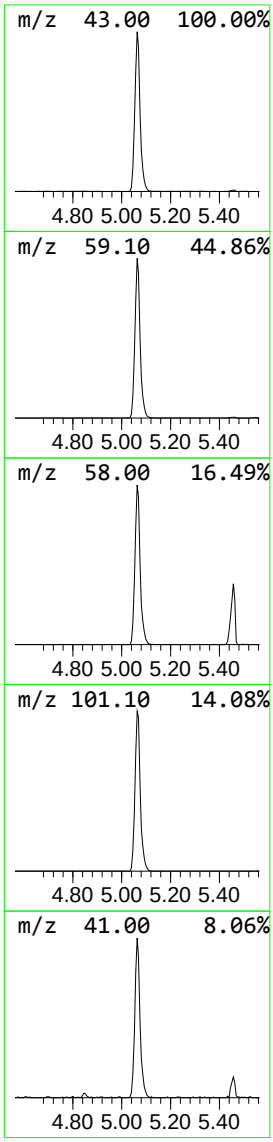
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	29.57 ng	1464910	1,4-Dichlorobenzene-d4	6.834

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	27
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	5-Aminovaleric acid	117	C5H11NO2	000660-88-8	9
5	Allyl acetate	100	C5H8O2	000591-87-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052523\
Data File : BF133492.D
Acq On : 25 May 2023 16:16
Operator : CG\JU
Sample : PB153012BL
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB153012BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

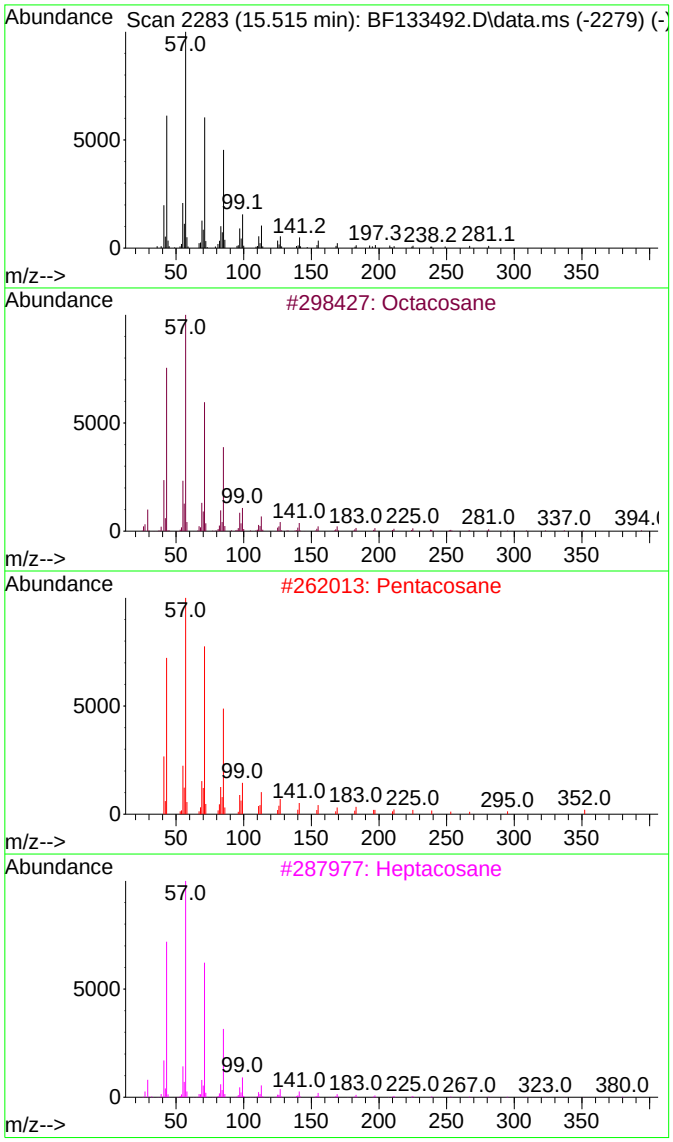
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

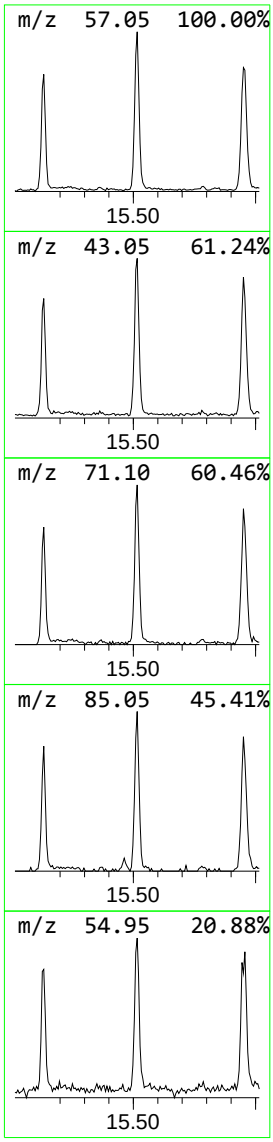
****

Peak Number 4 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.515	2.26 ng	160637	Perylene-d12	15.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Pentacosane	352	C25H52	000629-99-2	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Heneicosane	296	C21H44	000629-94-7	90
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052523\
Data File : BF133492.D
Acq On : 25 May 2023 16:16
Operator : CG\JU
Sample : PB153012BL
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB153012BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

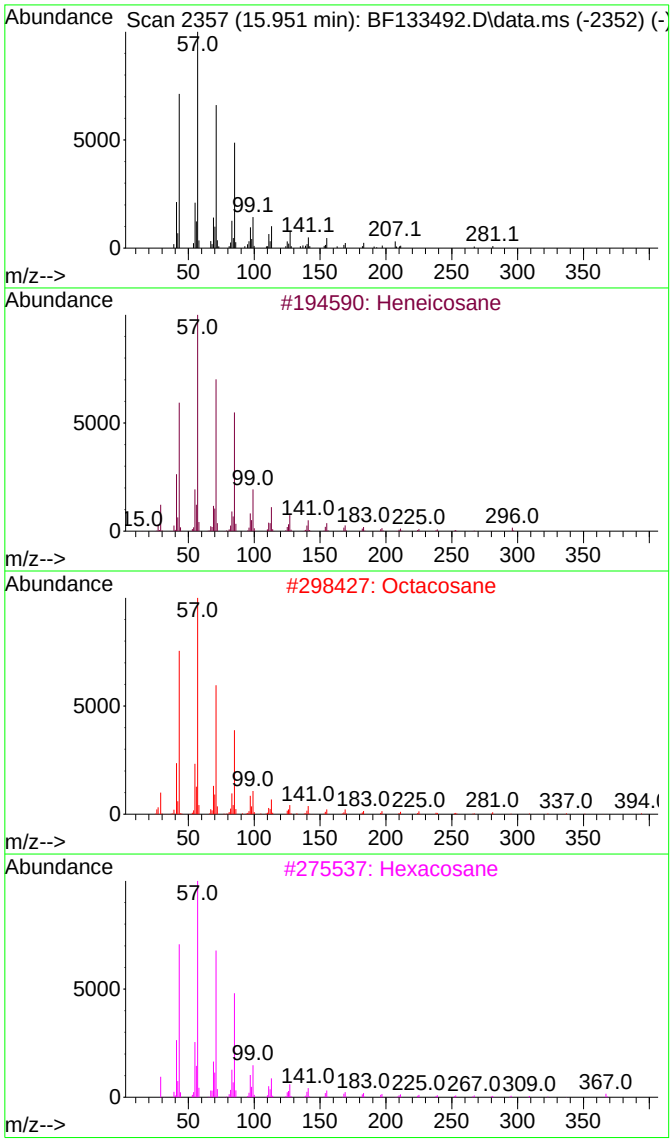
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

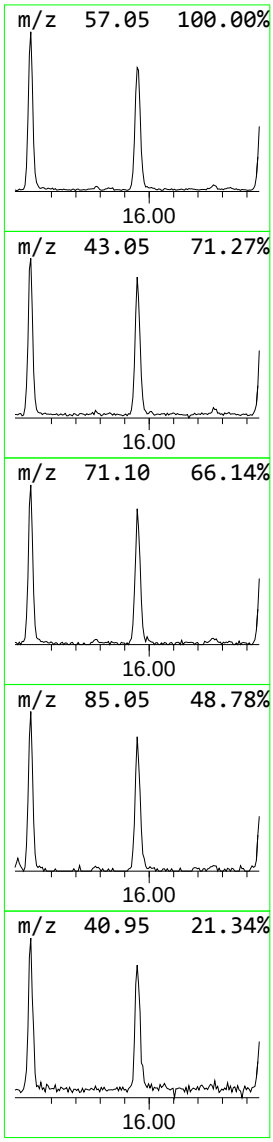
****

Peak Number 5 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.951	2.14 ng	151675	Perylene-d12	15.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052523\
Data File : BF133492.D
Acq On : 25 May 2023 16:16
Operator : CG\JU
Sample : PB153012BL
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB153012BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

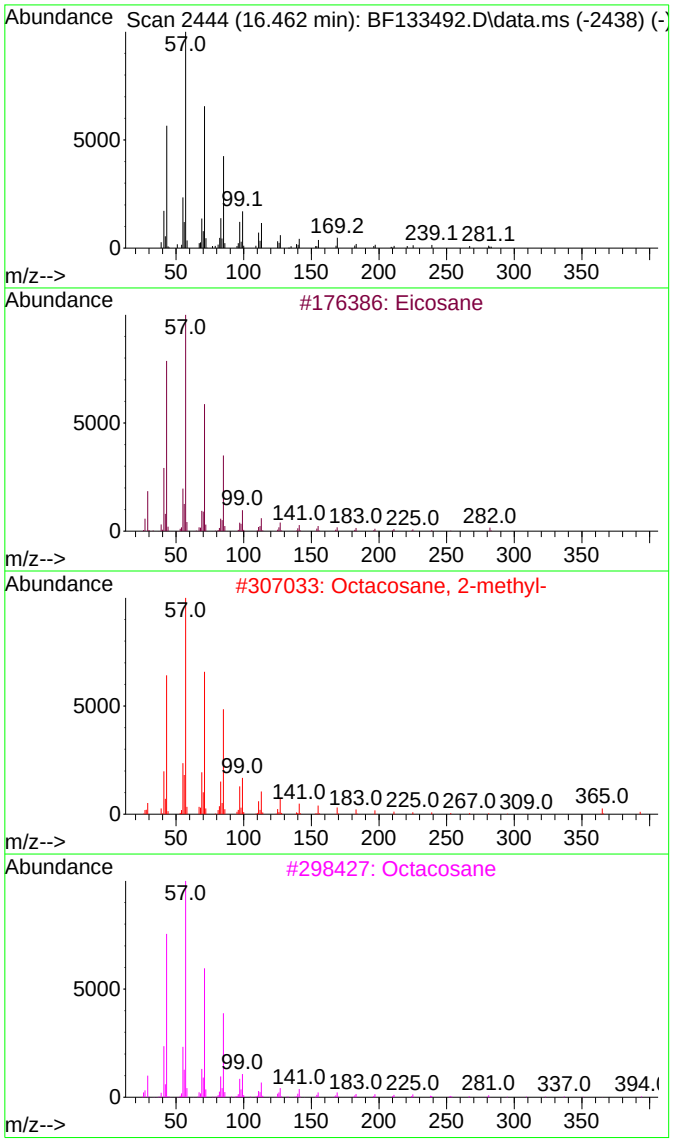
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

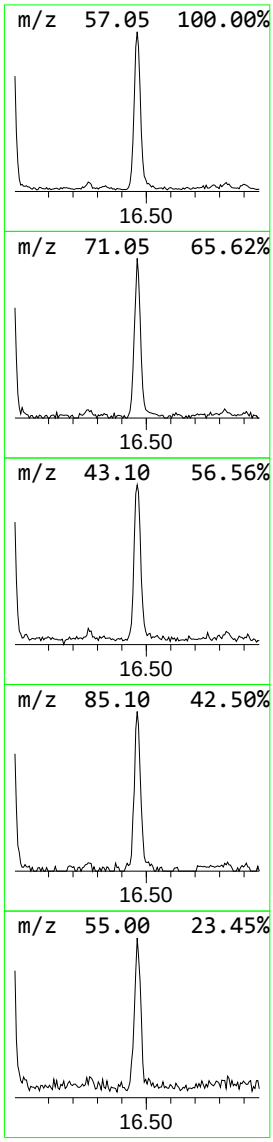
****

Peak Number 6 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.462	2.20 ng	156368	Perylene-d12	15.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3	Octacosane	394	C28H58	000630-02-4	90
4	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	90
5	Hentriacontane	437	C31H64	000630-04-6	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052523\
Data File : BF133492.D
Acq On : 25 May 2023 16:16
Operator : CG\JU
Sample : PB153012BL
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB153012BL

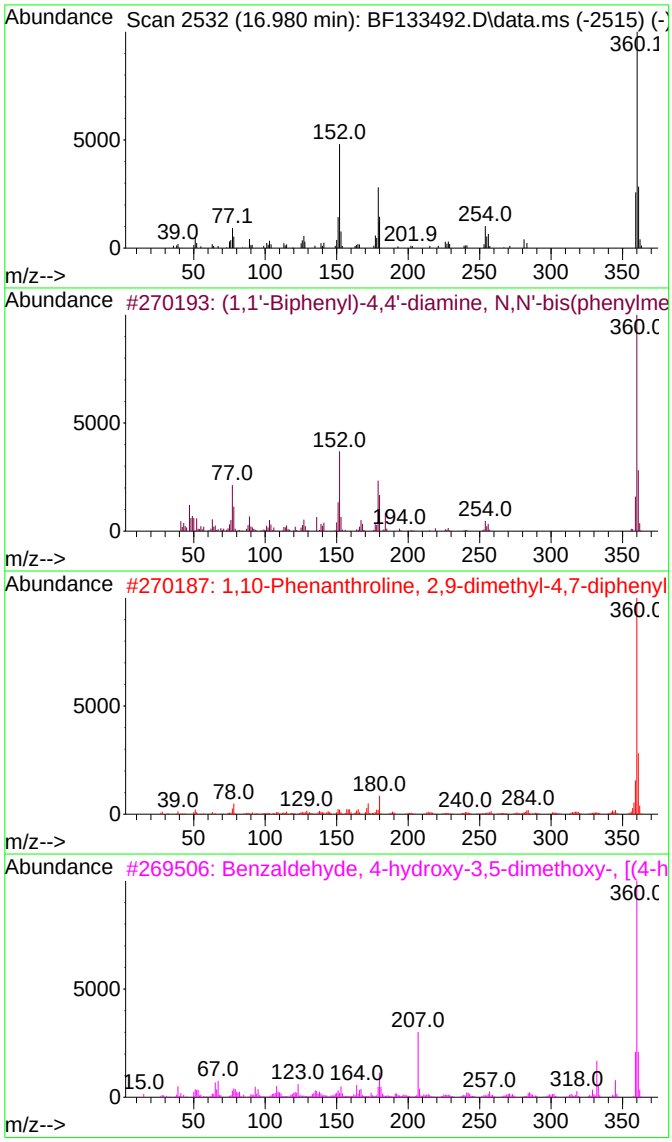
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

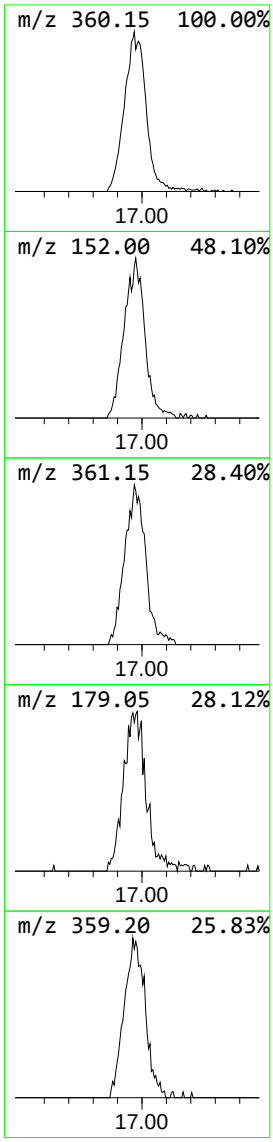
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.980	5.91 ng	419540	Perylene-d12	15.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1,1'-Biphenyl)-4,4'-diamine, N,...	360	C26H20N2	006311-48-4	87
2	1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	47
3	Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	47
4	Androst-4-ene-3,17-dione, 12-hyd...	360	C21H32N2O3	069688-31-9	43
5	1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13BO6	1000150-23-7	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052523\
Data File : BF133492.D
Acq On : 25 May 2023 16:16
Operator : CG\JU
Sample : PB153012BL
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB153012BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.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...	2.157	2.6	ng	131286	1	6.834	990900	20.0
3-Penten-2-one,...	4.434	7.9	ng	391398	1	6.834	990900	20.0
2-Pentanone, 4-...	5.063	29.6	ng	1464910	1	6.834	990900	20.0
Octacosane	15.515	2.3	ng	160637	6	15.463	1418890	20.0
Heneicosane	15.951	2.1	ng	151675	6	15.463	1418890	20.0
Eicosane	16.462	2.2	ng	156368	6	15.463	1418890	20.0
(1,1'-Biphenyl)...	16.980	5.9	ng	419540	6	15.463	1418890	20.0