LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122821\
Data File : BF126391.D
Acq On : 28 Dec 2021 20:20
Operator : JU/CG
Sample : M5115-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

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-BF121521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126391.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	12	17	26	rVB2	46595	76107	2.36%	0.359%
2	3.246	192	197	207	rVB	71151	130716	4.06%	0.617%
3	3.857	297	301	306	rVB	37836	47844	1.49%	0.226%
4	4.387	387	391	396	rBV	40612	48295	1.50%	0.228%
5	5.010	492	497	504	rBV	530122	604054	18.76%	2.850%
6	5.422	562	567	570	rBV	2303428	2203072	68.43%	10.396%
7	5.822	631	635	640	rBV	188494	166717	5.18%	0.787%
8	5.904	646	649	657	rBV	39135	84019	2.61%	0.396%
9	6.434	735	739	743	rBV	1531078	1404674	43.63%	6.628%
10	6.810	797	803	806	rBV	930432	860095	26.72%	4.059%
11	6.869	810	813	821	rBV4	35457	56902	1.77%	0.269%
12	7.216	868	872	875	rBV4	33543	48544	1.51%	0.229%
13	7.375	893	899	902	rBV	2521425	2711303	84.22%	12.794%
14	7.422	904	907	913	rVV	36551	56638	1.76%	0.267%
15	7.486	913	918	926	rVB5	41578	81424	2.53%	0.384%
16	7.881	981	985	990	rBV4	29418	42378	1.32%	0.200%
17	8.010	1003	1007	1009	rBV3	28490	39231	1.22%	0.185%
18	8.092	1017	1021	1024	rBV	1263738	1092018	33.92%	5.153%
19	8.228	1035	1044	1050	rBV10	34524	89142	2.77%	0.421%
20	8.292	1050	1055	1059	rBV4	40875	75521	2.35%	0.356%
21	8.369	1063	1068	1074	rVB2	74419	115274	3.58%	0.544%
22	8.463	1081	1084	1087	rBV2	43434	57894	1.80%	0.273%
23	8.522	1087	1094	1100	rVB4	184437	325416	10.11%	1.536%
24	8.598	1105	1107	1110	rVB	60984	45696	1.42%	0.216%
25	8.851	1147	1150	1157	rVB2	45421	57350	1.78%	0.271%
26	9.075	1183	1188	1190	rBV2	42387	59072	1.83%	0.279%
27	9.122	1193	1196	1199	rVV2	42972	65638	2.04%	0.310%
28	9.175	1199	1205	1208	rVB	3207652	3219446	100.00%	15.192%
29	9.463	1251	1254	1257	rBV2	32020	37030	1.15%	0.175%
30	9.616	1277	1280	1287	rBV	152109	206641	6.42%	0.975%
31	9.757	1300	1304	1307	rBV	105981	105615	3.28%	0.498%
32	9.845	1315	1319	1323	rVB	1070590	864578	26.85%	4.080%
33	10.445	1418	1421	1425	rBV	73659	82150	2.55%	0.388%
34	10.633	1449	1453	1464	rBV	1727039	1692474	52.57%	7.986%
35	10.974	1507	1511	1516	rBV2	52362	78084	2.43%	0.368%
36	11.221	1551	1553	1557	rVB	40546	33644	1.05%	0.159%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122821\
Data File : BF126391.D
Acq On : 28 Dec 2021 20:20
Operator : JU/CG
Sample : M5115-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

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-BF121521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.333	1568	1572	1575	rBV	754993	688255	21.38%	3.248%
38	11.863	1659	1662	1671	rBV2	91860	108177	3.36%	0.510%
39	12.651	1793	1796	1803	rBV7	21247	42012	1.30%	0.198%
40	12.921	1837	1842	1845	rBV	2307524	2050132	63.68%	9.674%
41	13.468	1931	1935	1940	rBV2	34855	46720	1.45%	0.220%
42	13.845	1995	1999	2013	rVV2	99308	195356	6.07%	0.922%
43	13.968	2016	2020	2025	rVB	590296	514459	15.98%	2.428%
44	15.415	2261	2266	2271	rBV	363092	446120	13.86%	2.105%
45	15.886	2342	2346	2352	rBV3	23547	32872	1.02%	0.155%
46	16.139	2383	2389	2396	rBV9	23347	63467	1.97%	0.299%
47	16.956	2524	2528	2538	rVB8	15332	40126	1.25%	0.189%

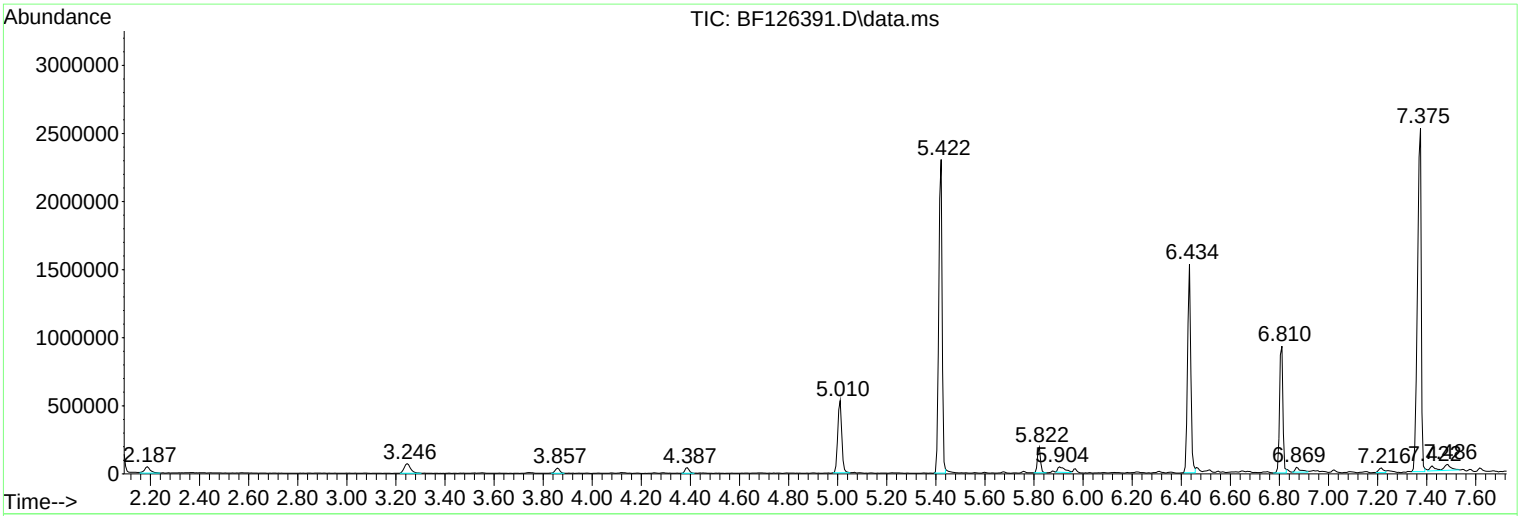
Sum of corrected areas: 21192392

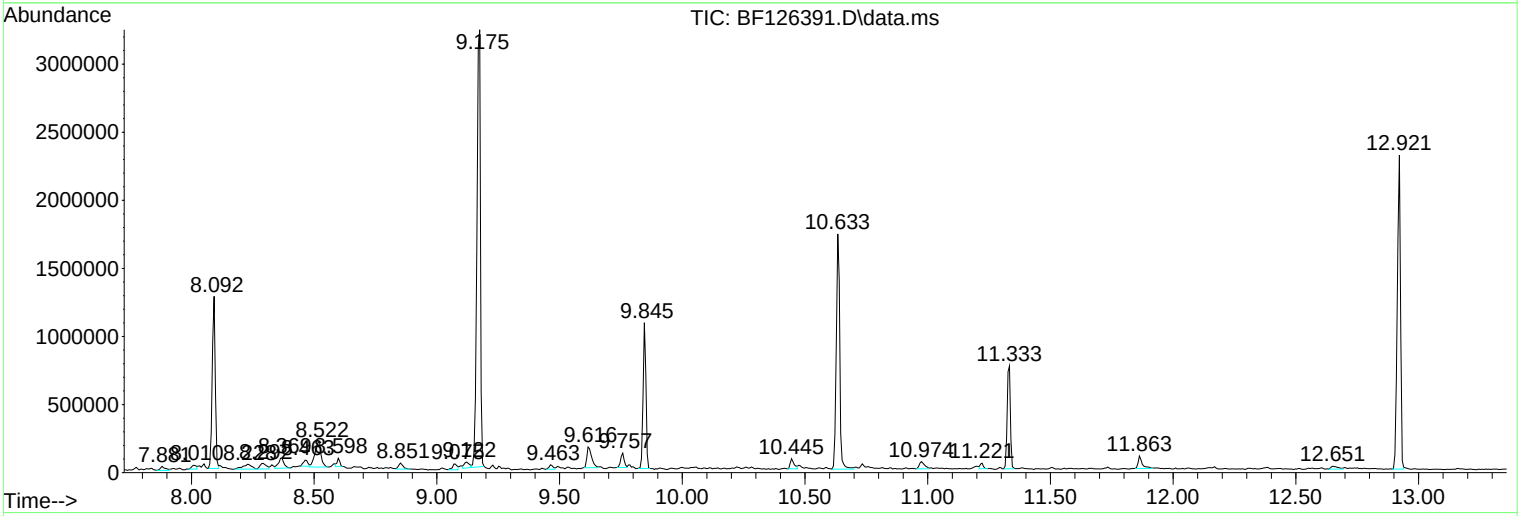
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122821\
Data File : BF126391.D
Acq On : 28 Dec 2021 20:20
Operator : JU/CG
Sample : M5115-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

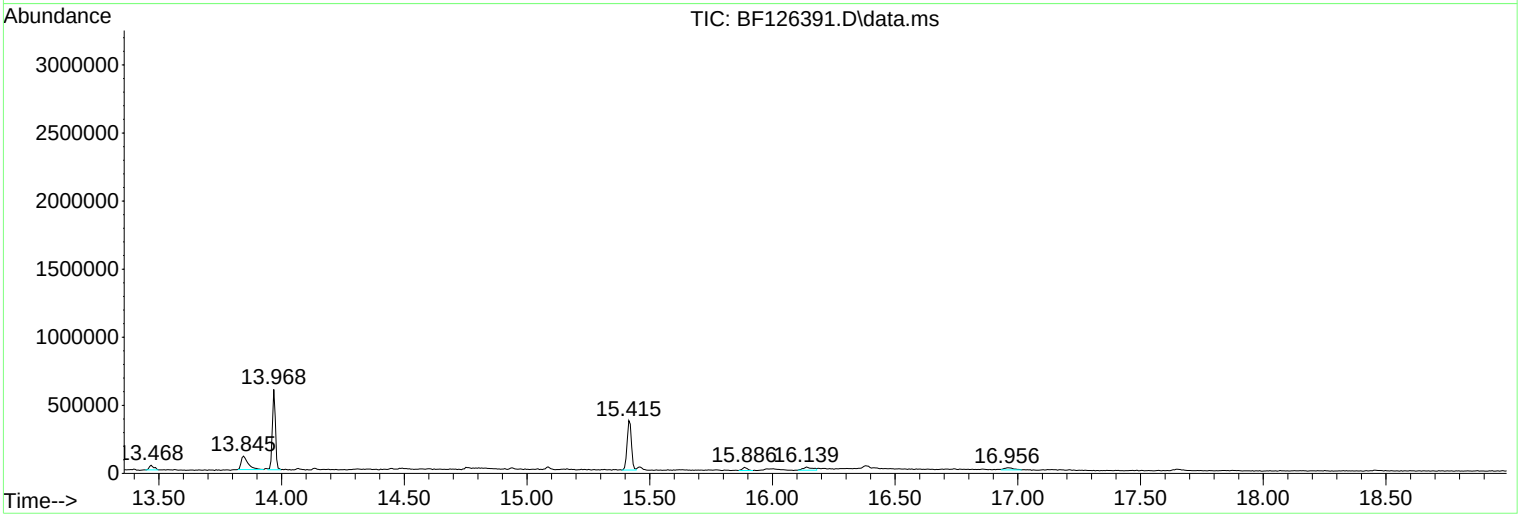
Instrument :
BNA_F
ClientSampleId :
MW-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.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\BF122821\
Data File : BF126391.D
Acq On : 28 Dec 2021 20:20
Operator : JU/CG
Sample : M5115-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

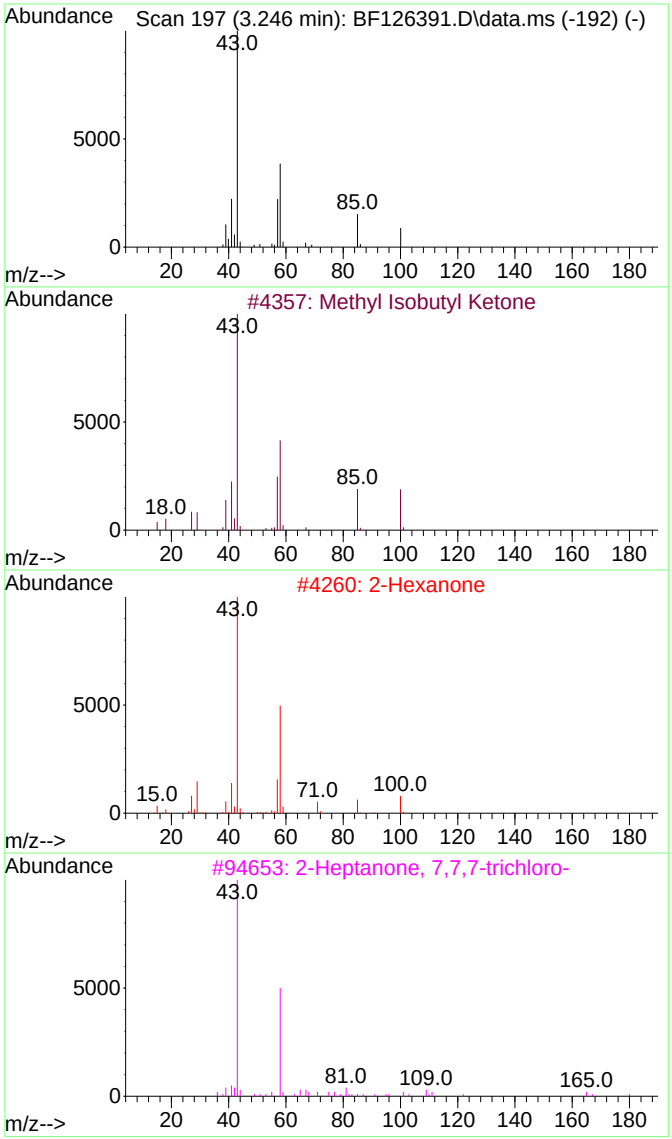
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

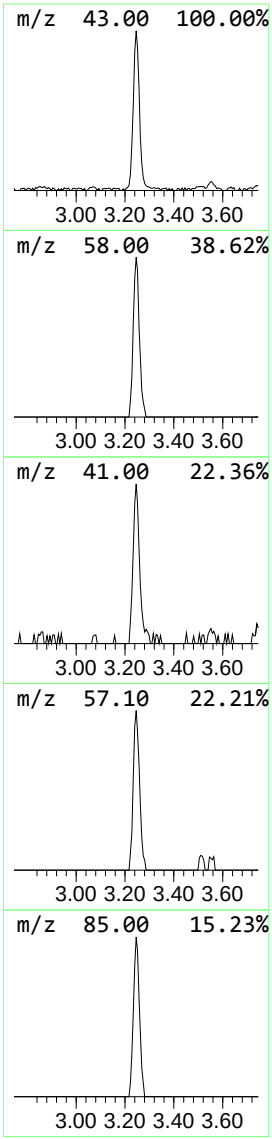
****

Peak Number 1 Methyl Isobutyl Ketone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.246	3.04 ng	130716	1,4-Dichlorobenzene-d4	6.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl Isobutyl Ketone	100	C6H12O	000108-10-1	90
2	2-Hexanone	100	C6H12O	000591-78-6	78
3	2-Heptanone, 7,7,7-trichloro-	216	C7H11Cl3O	154264-40-1	42
4	Pentanal, 2-methyl-	100	C6H12O	000123-15-9	33
5	Octane	114	C8H18	000111-65-9	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122821\
Data File : BF126391.D
Acq On : 28 Dec 2021 20:20
Operator : JU/CG
Sample : M5115-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

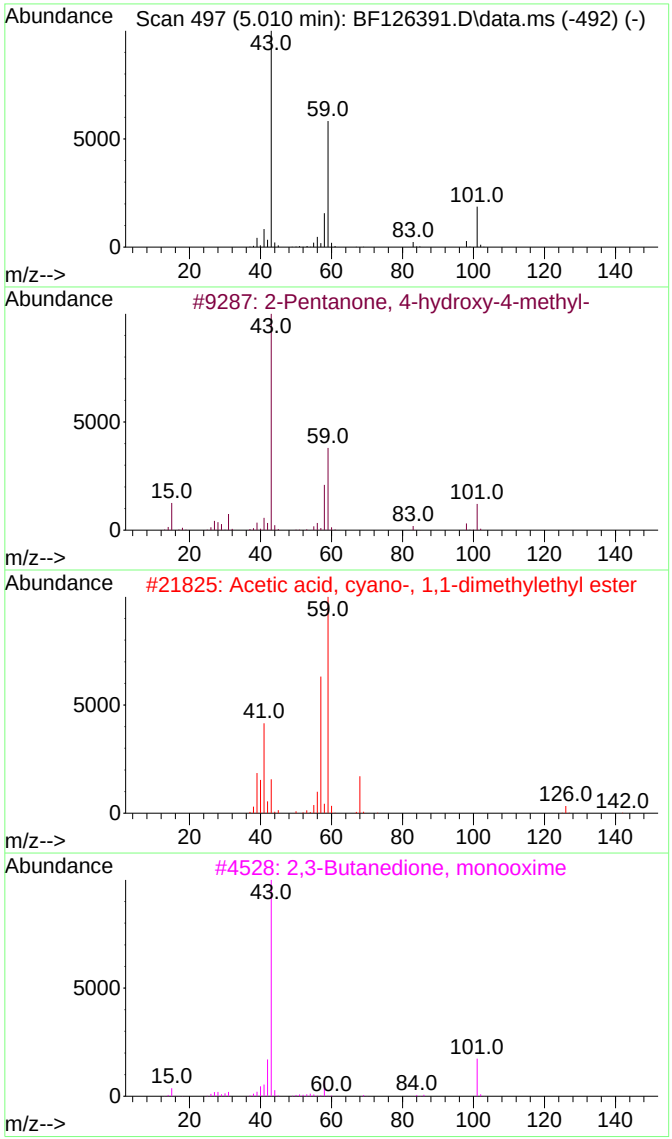
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

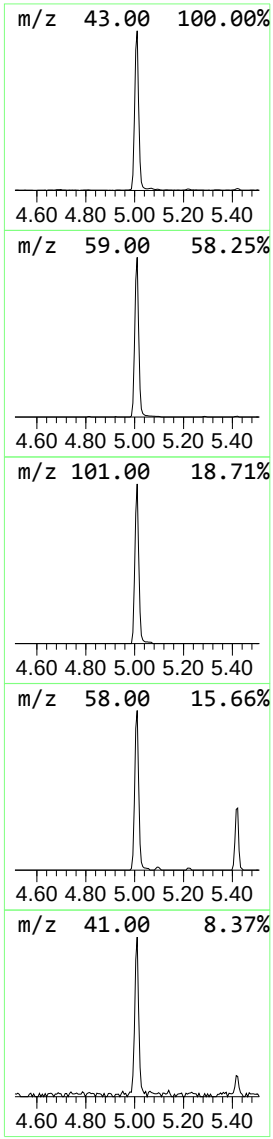
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.010	14.05 ng	604054	1,4-Dichlorobenzene-d4	6.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122821\
Data File : BF126391.D
Acq On : 28 Dec 2021 20:20
Operator : JU/CG
Sample : M5115-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

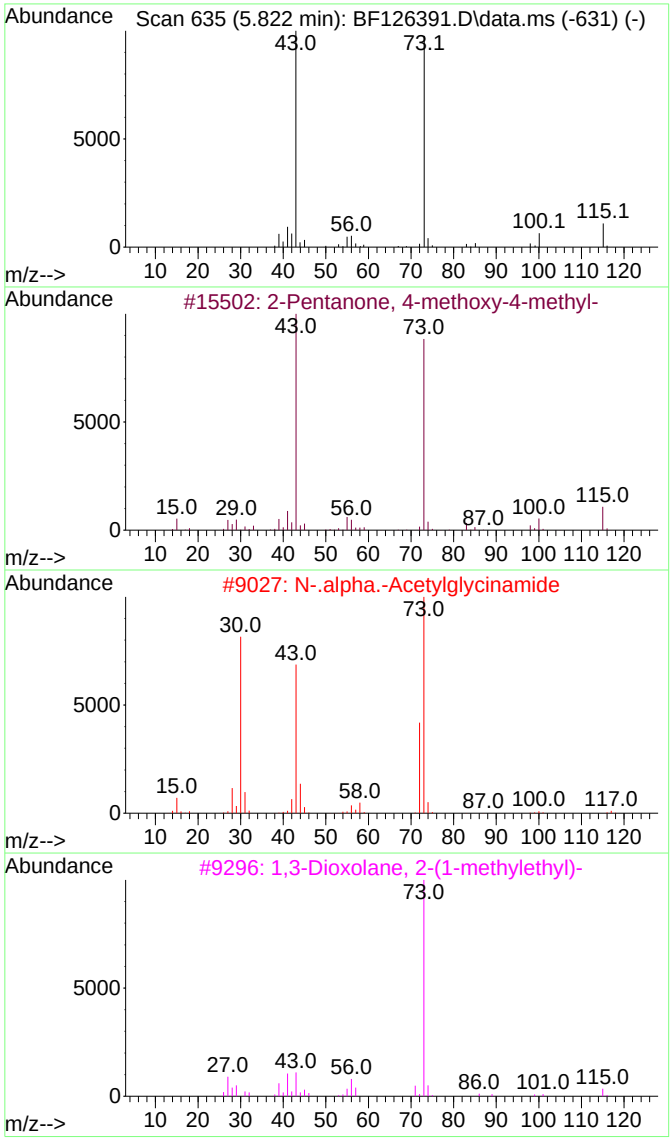
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

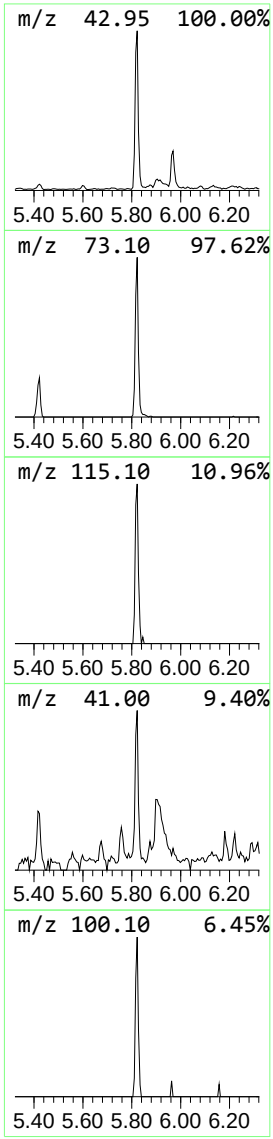
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.822	3.88 ng	166717	1,4-Dichlorobenzene-d4	6.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	47
3	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	27
4	N-Formylmorpholine	115	C5H9NO2	004394-85-8	10
5	Acetamide, N-butyl-	115	C6H13NO	001119-49-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122821\
Data File : BF126391.D
Acq On : 28 Dec 2021 20:20
Operator : JU/CG
Sample : M5115-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

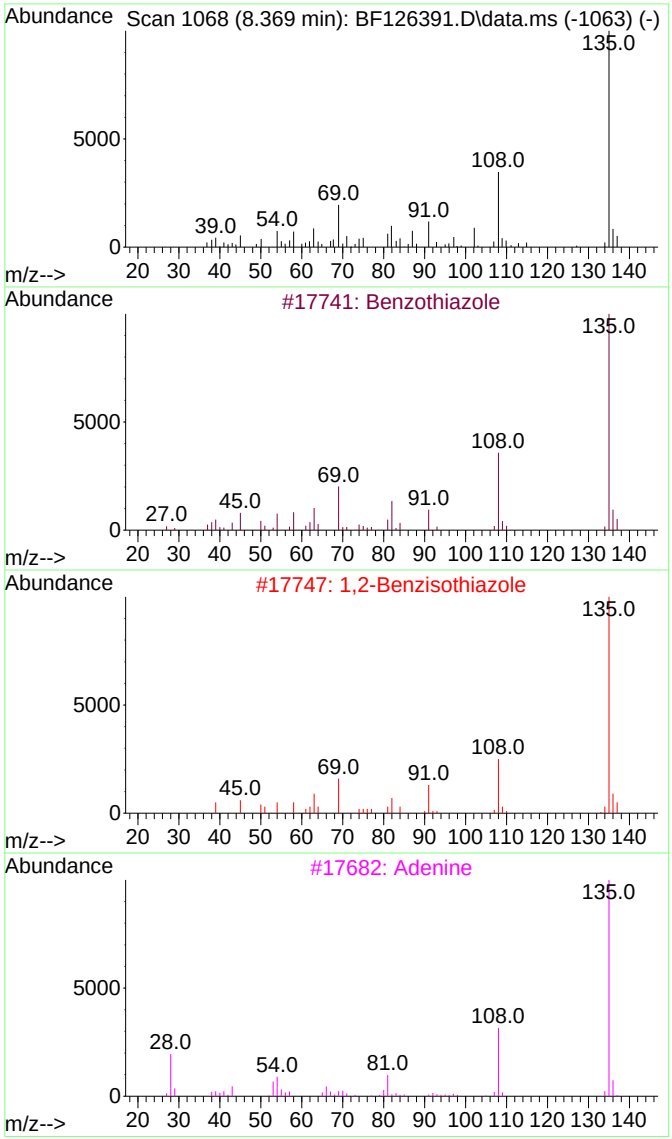
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

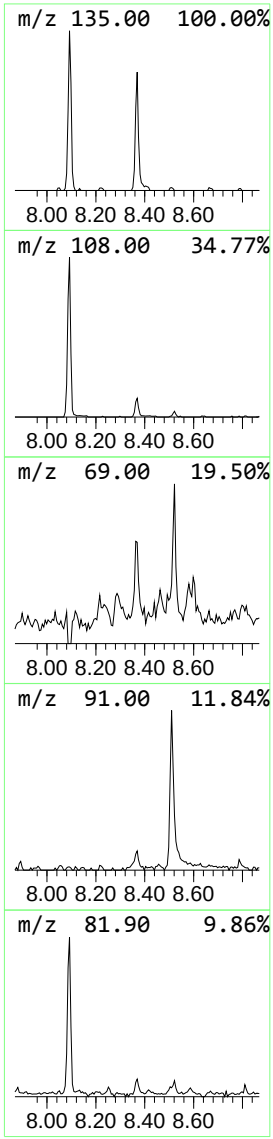
****

Peak Number 4 Benzothiazole Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.369	2.11 ng	115274	Naphthalene-d8	8.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole	135	C7H5NS	000095-16-9	94
2	1,2-Benzisothiazole	135	C7H5NS	000272-16-2	90
3	Adenine	135	C5H5N5	000073-24-5	64
4	1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	002380-63-4	59
5	1H-Indole, 5-fluoro-	135	C8H6FN	000399-52-0	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122821\
Data File : BF126391.D
Acq On : 28 Dec 2021 20:20
Operator : JU/CG
Sample : M5115-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

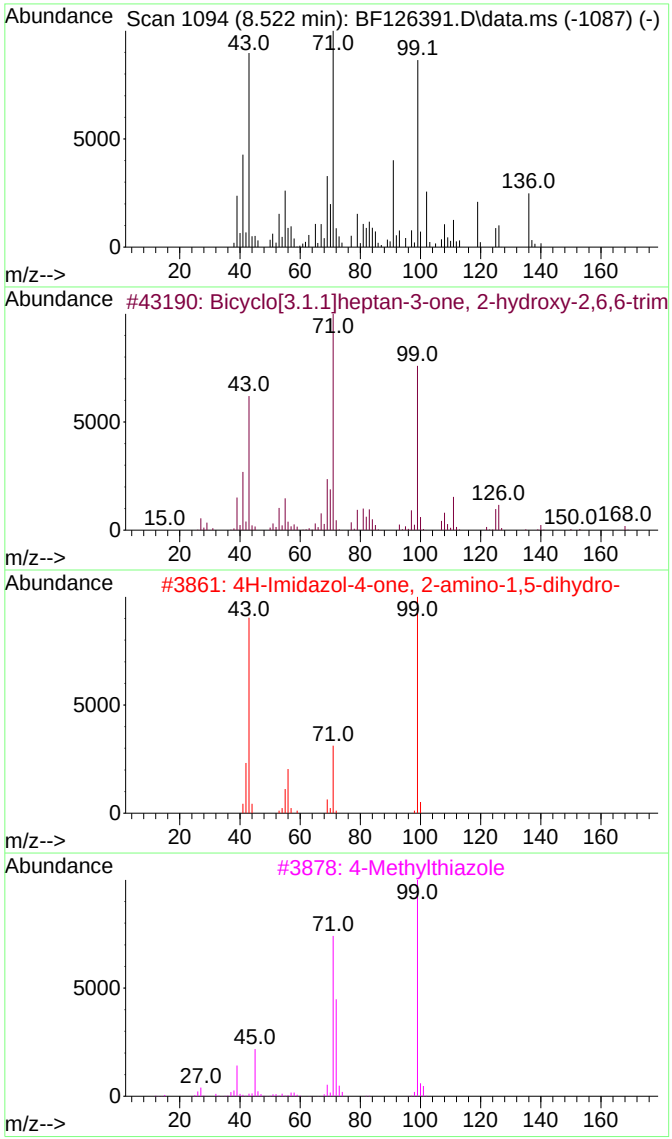
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

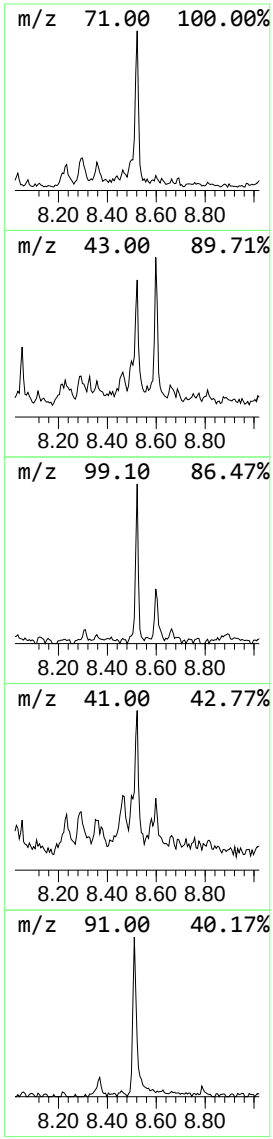
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Bicyclo[3.1.1]heptan-3-one,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.522	5.96 ng	325416	Naphthalene-d8	8.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.1]heptan-3-one, 2-hy...	168	C10H16O2	010136-65-9	58
2	4H-Imidazol-4-one, 2-amino-1,5-d...	99	C3H5N3O	000503-86-6	47
3	4-Methylthiazole	99	C4H5NS	000693-95-8	47
4	2-Ethylbutyric acid, 2-formylphe...	220	C13H16O3	1000369-96-4	47
5	Pentanoic acid, 2-methyl-, anhyd...	214	C12H22O3	063169-61-9	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122821\
Data File : BF126391.D
Acq On : 28 Dec 2021 20:20
Operator : JU/CG
Sample : M5115-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

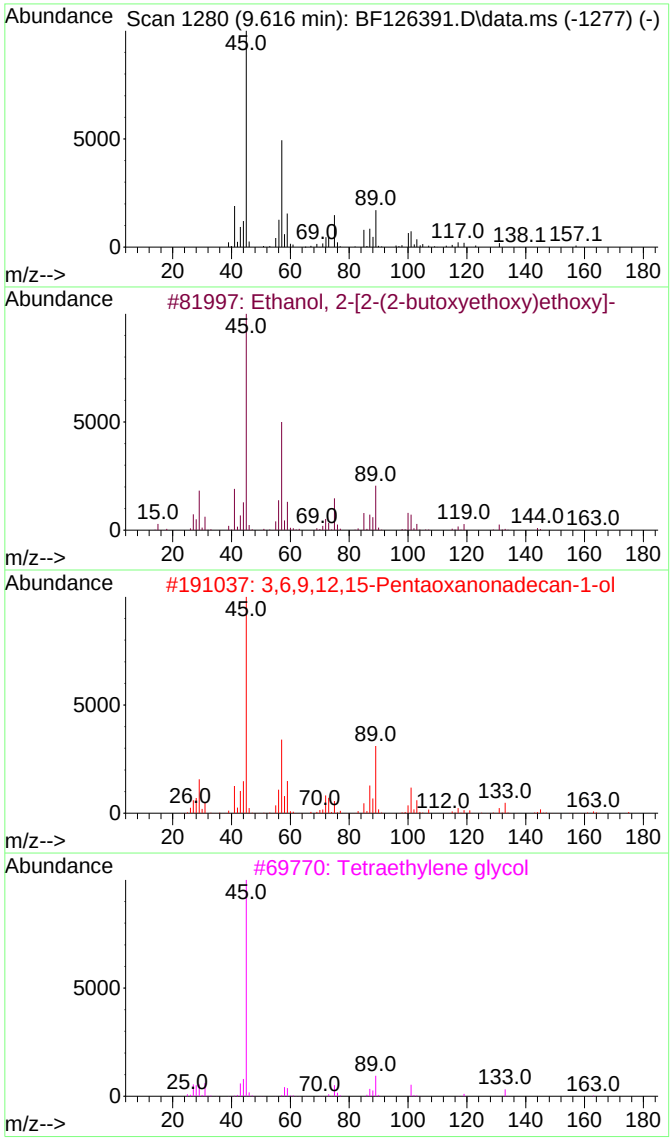
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

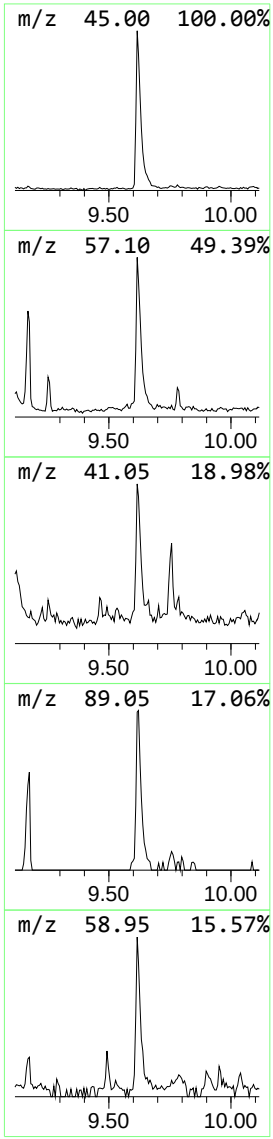
****

Peak Number 6 Ethanol, 2-[2-(2-butoxyetho... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.616	4.78 ng	206641	Acenaphthene-d10	9.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	91
2	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	78
3	Tetraethylene glycol	194	C8H18O5	000112-60-7	72
4	Hexaethylene glycol	282	C12H26O7	002615-15-8	64
5	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122821\
Data File : BF126391.D
Acq On : 28 Dec 2021 20:20
Operator : JU/CG
Sample : M5115-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

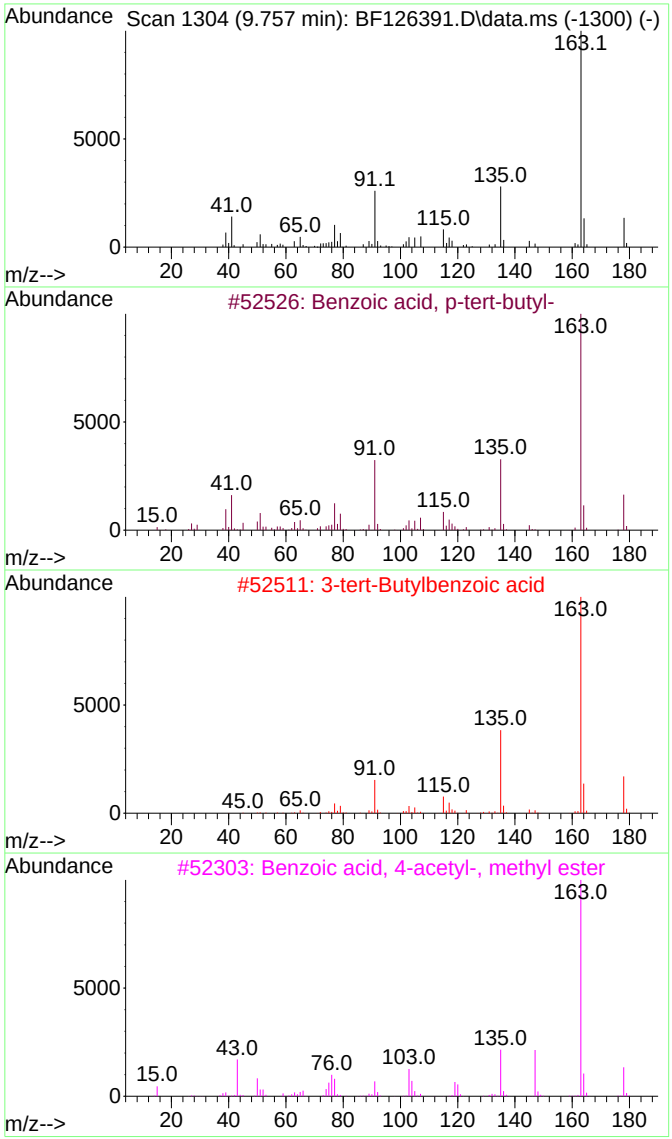
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

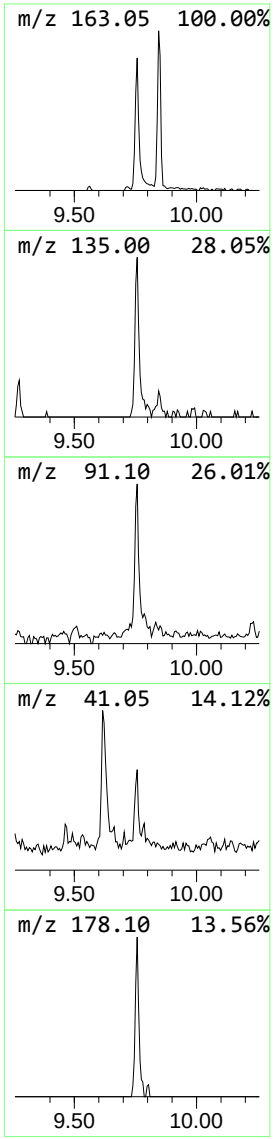
****

Peak Number 7 Benzoic acid, p-tert-butyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.757	2.44 ng	105615	Acenaphthene-d10	9.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	96
2	3-tert-Butylbenzoic acid	178	C11H14O2	007498-54-6	87
3	Benzoic acid, 4-acetyl-, methyl ...	178	C10H10O3	003609-53-8	72
4	6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	72
5	Benzaldehyde, 5-(1,1-dimethyleth...	178	C11H14O2	002725-53-3	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122821\
Data File : BF126391.D
Acq On : 28 Dec 2021 20:20
Operator : JU/CG
Sample : M5115-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

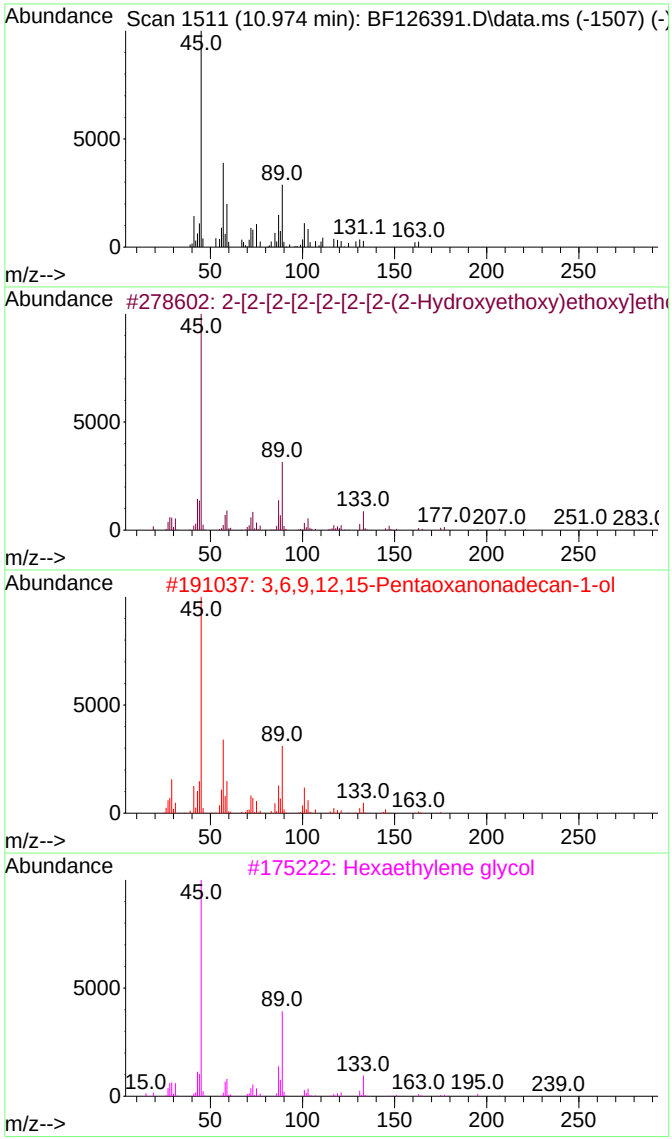
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

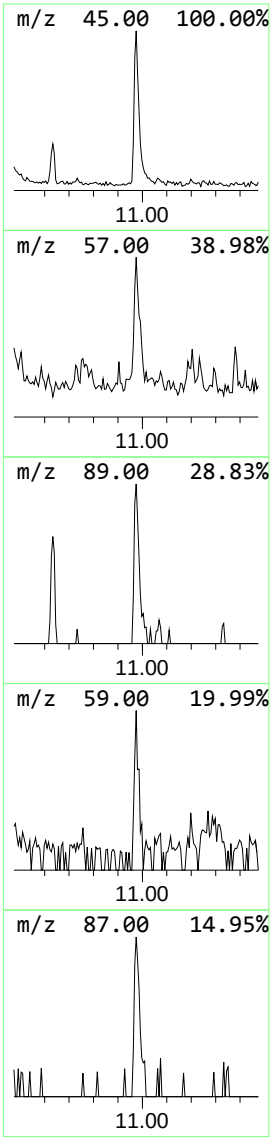
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2-[2-[2-[2-[2-[2-[2-(2-Hydr... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.974	2.27 ng	78084	Phenanthrene-d10	11.333

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	72
2	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	72
3	Hexaethylene glycol	282	C12H26O7	002615-15-8	64
4	Tetraethylene glycol	194	C8H18O5	000112-60-7	59
5	Heptaethylene glycol	326	C14H30O8	005617-32-3	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122821\
Data File : BF126391.D
Acq On : 28 Dec 2021 20:20
Operator : JU/CG
Sample : M5115-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

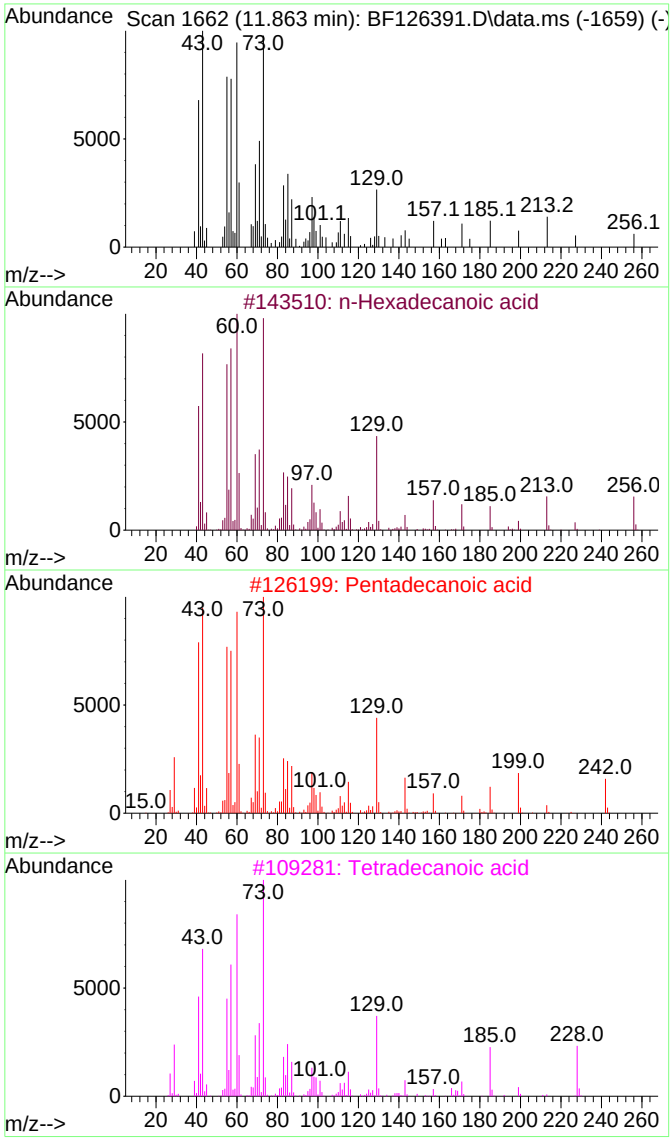
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

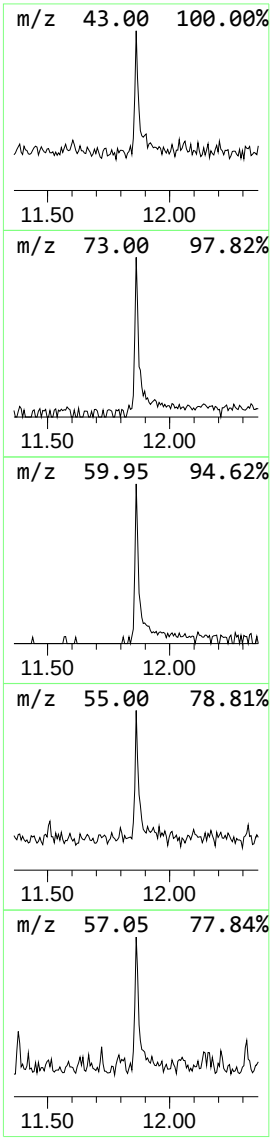
****

Peak Number 9 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	3.14 ng	108177	Phenanthrene-d10	11.333

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
4	Dodecanoic acid	200	C12H24O2	000143-07-7	53
5	5-Methyloctanoic acid	158	C9H18O2	060218-42-0	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122821\
Data File : BF126391.D
Acq On : 28 Dec 2021 20:20
Operator : JU/CG
Sample : M5115-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

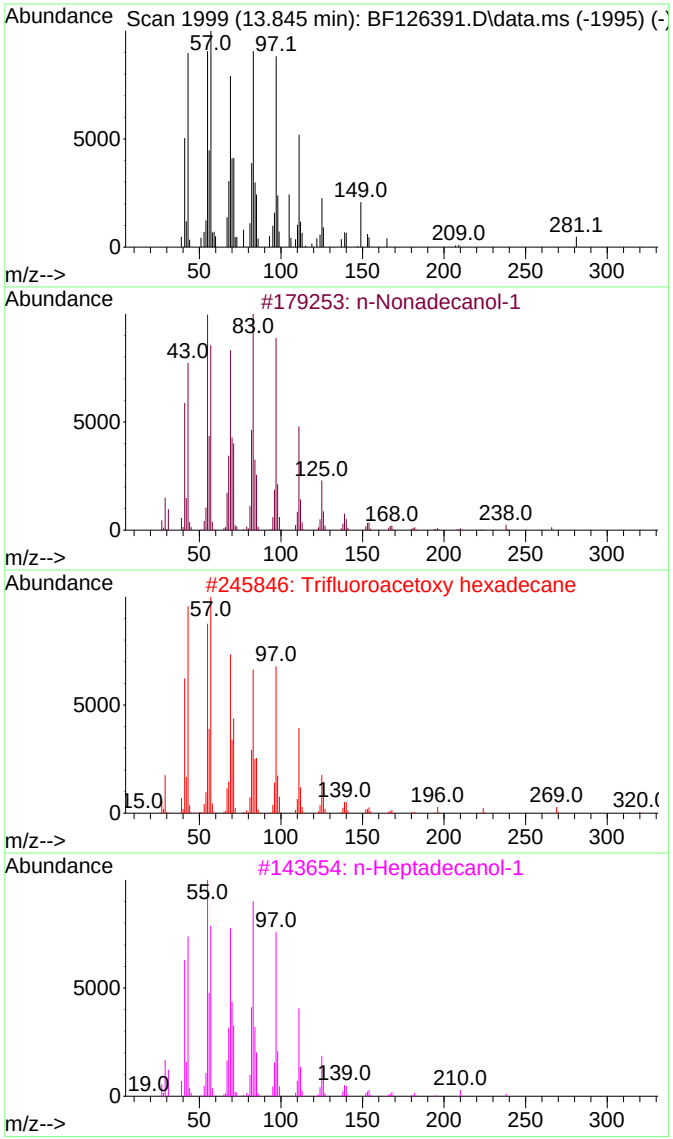
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

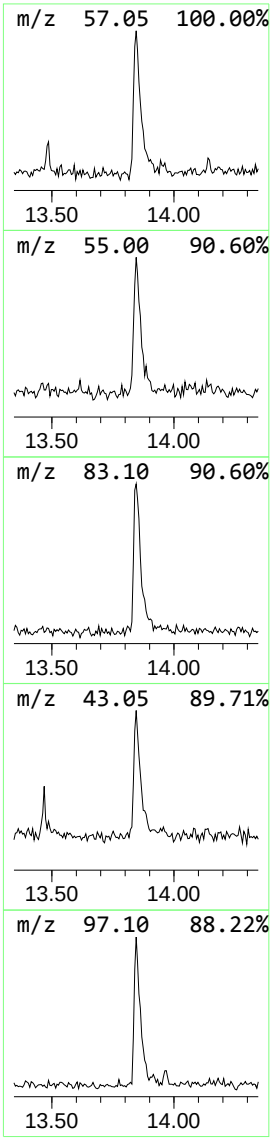
****

Peak Number 10 n-Nonadecanol-1 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	7.59 ng	195356	Chrysene-d12	13.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
3	n-Heptadecanol-1	256	C17H36O	001454-85-9	95
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Behenic alcohol	326	C22H46O	000661-19-8	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122821\
Data File : BF126391.D
Acq On : 28 Dec 2021 20:20
Operator : JU/CG
Sample : M5115-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

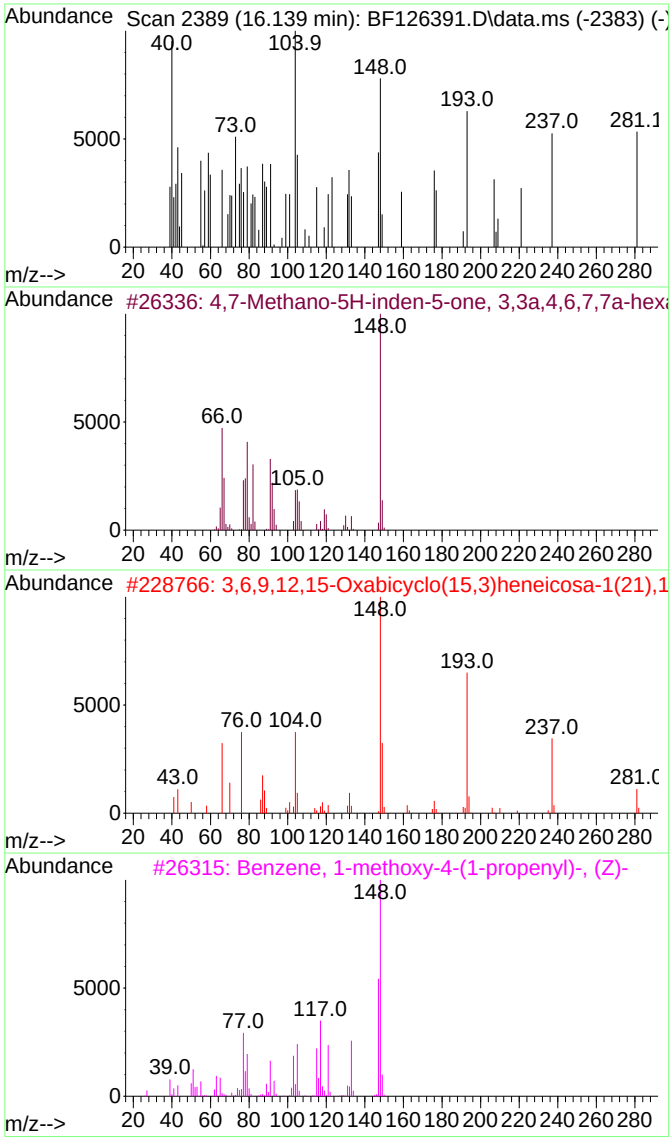
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

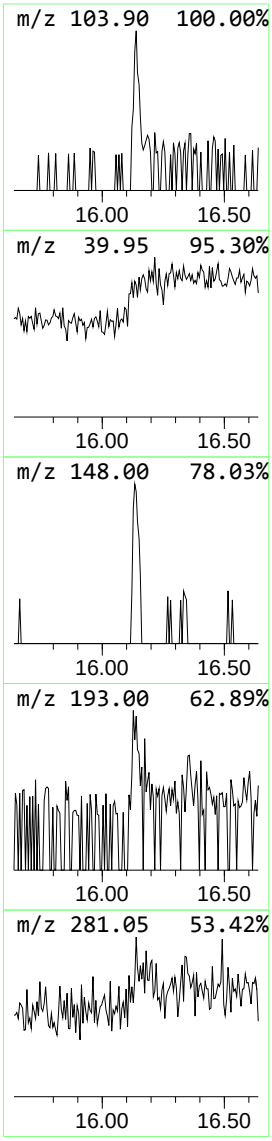
****

Peak Number 11 unknown16.139 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.139	2.85 ng	63467	Perylene-d12	15.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,7-Methano-5H-inden-5-one, 3,3a...	148	C10H12O	014888-58-5	30
2	3,6,9,12,15-Oxabicyclo(15,3)hene...	324	C16H20O7	065745-83-7	23
3	Benzene, 1-methoxy-4-(1-propenyl...	148	C10H12O	025679-28-1	11
4	4-Hydroxy-3-(methylamino)benzoni...	148	C8H8N2O	1000435-54-8	11
5	Silane, 1,6-heptadiyne-1,7-diylb...	236	C13H24Si2	041268-43-3	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122821\
Data File : BF126391.D
Acq On : 28 Dec 2021 20:20
Operator : JU/CG
Sample : M5115-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.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
Methyl Isobutyl...	3.246	3.0	ng	130716	1	6.810	860095	20.0
2-Pentanone, 4-...	5.010	14.1	ng	604054	1	6.810	860095	20.0
2-Pentanone, 4-...	5.822	3.9	ng	166717	1	6.810	860095	20.0
Benzothiazole	8.369	2.1	ng	115274	2	8.092	1092020	20.0
Bicyclo[3.1.1]h...	8.522	6.0	ng	325416	2	8.092	1092020	20.0
Ethanol, 2-[2-(...	9.616	4.8	ng	206641	3	9.845	864578	20.0
Benzoic acid, p...	9.757	2.4	ng	105615	3	9.845	864578	20.0
2-[2-[2-[2-[2-[...	10.974	2.3	ng	78084	4	11.333	688255	20.0
n-Hexadecanoic ...	11.863	3.1	ng	108177	4	11.333	688255	20.0
n-Nonadecanol-1	13.845	7.6	ng	195356	5	13.968	514459	20.0
unknown16.139	16.139	2.9	ng	63467	6	15.415	446120	20.0