Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022522\
Data File : BF127085.D
Acq On : 25 Feb 2022 21:57
Operator : CG\JU
Sample : N1655-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UNK-SOUTH

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-BF021622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127085.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.122	478	482	490	rBV	53462	62875	2.71%	0.368%
2	5.387	524	527	531	rBV	74162	76638	3.30%	0.449%
3	5.493	542	545	546	rBV	35285	28168	1.21%	0.165%
4	5.522	546	550	553	rVB	2212687	1935382	83.42%	11.327%
5	6.357	690	692	695	rBV	74985	64639	2.79%	0.378%
6	6.387	695	697	701	rVB2	34009	30888	1.33%	0.181%
7	6.528	716	721	727	rVB	2111420	2033733	87.66%	11.903%
8	6.722	751	754	763	rBV2	69095	71228	3.07%	0.417%
9	6.898	781	784	788	rVB	787880	626783	27.02%	3.668%
10	6.951	789	793	796	rBV	30051	30918	1.33%	0.181%
11	7.016	800	804	809	rBV	33661	40100	1.73%	0.235%
12	7.081	812	815	818	rVB	94055	78403	3.38%	0.459%
13	7.145	823	826	828	rBV	93403	82755	3.57%	0.484%
14	7.163	828	829	835	rVB2	41956	34943	1.51%	0.205%
15	7.216	835	838	840	rBV	84556	70615	3.04%	0.413%
16	7.287	845	850	854	rBV	33716	36828	1.59%	0.216%
17	7.434	871	875	876	rBV	203480	181919	7.84%	1.065%
18	7.463	876	880	883	rVV	1646716	1407066	60.65%	8.235%
19	7.534	887	892	897	rBV3	29592	36090	1.56%	0.211%
20	7.663	911	914	917	rVB	89330	70518	3.04%	0.413%
21	7.781	930	934	939	rBV	30954	27066	1.17%	0.158%
22	7.851	944	946	950	rVB2	60032	53703	2.31%	0.314%
23	7.916	950	957	960	rBV2	129286	110991	4.78%	0.650%
24	8.081	982	985	990	rBV	28626	35418	1.53%	0.207%
25	8.181	998	1002	1005	rBV	938194	835964	36.03%	4.893%
26	9.257	1181	1185	1188	rBV	2807530	2319947	100.00%	13.578%
27	9.939	1298	1301	1305	rBV	1026348	875988	37.76%	5.127%
28	10.733	1432	1436	1439	rBV	1718668	1475072	63.58%	8.633%
29	11.433	1551	1555	1558	rBV	1062674	871929	37.58%	5.103%
30	11.945	1639	1642	1647	rBV	53900	48927	2.11%	0.286%
31	13.022	1820	1825	1828	rBV	2181252	1985066	85.57%	11.618%
32	13.939	1977	1981	1992	rVB6	51267	109126	4.70%	0.639%
33	14.074	2001	2004	2008	rBV	564901	511491	22.05%	2.994%
34	15.192	2191	2194	2198	rBV2	36883	45738	1.97%	0.268%
35	15.574	2254	2259	2266	rVB2	457647	600290	25.88%	3.513%
36	16.039	2334	2338	2343	rVB3	39030	58417	2.52%	0.342%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022522\
Data File : BF127085.D
Acq On : 25 Feb 2022 21:57
Operator : CG\JU
Sample : N1655-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UNK-SOUTH

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-BF021622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.562	2424	2427	2436	rVB4	28587	54005	2.33%	0.316%
38	17.439	2573	2576	2583	rVB7	35534	66225	2.85%	0.388%

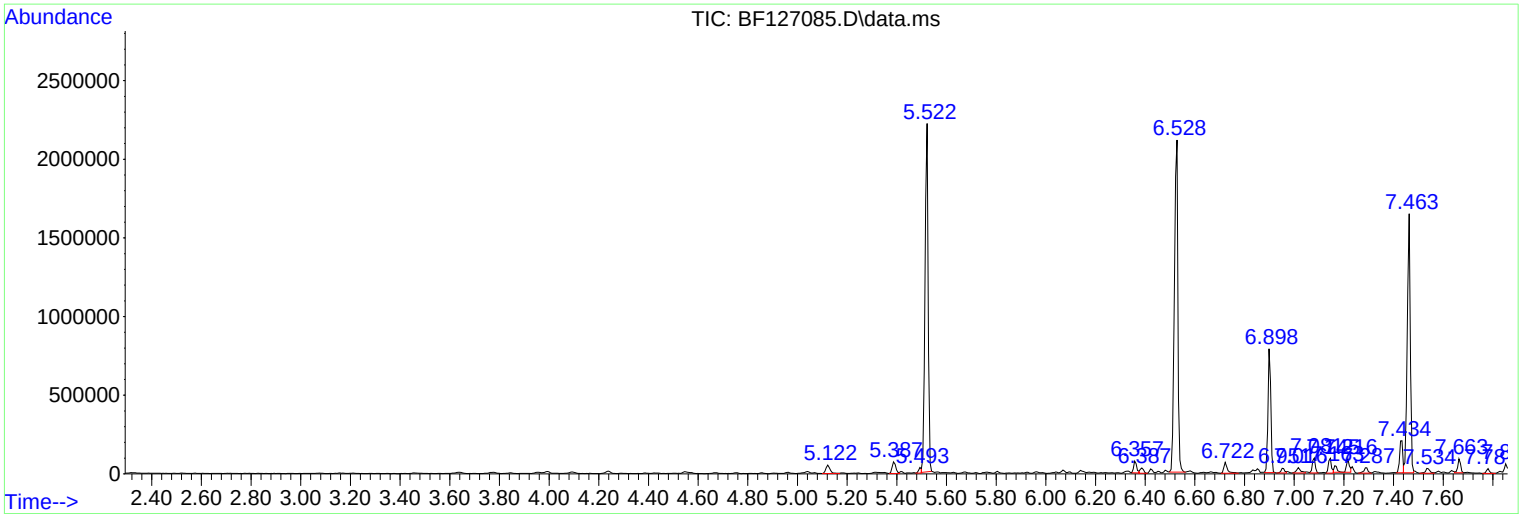
Sum of corrected areas: 17085852

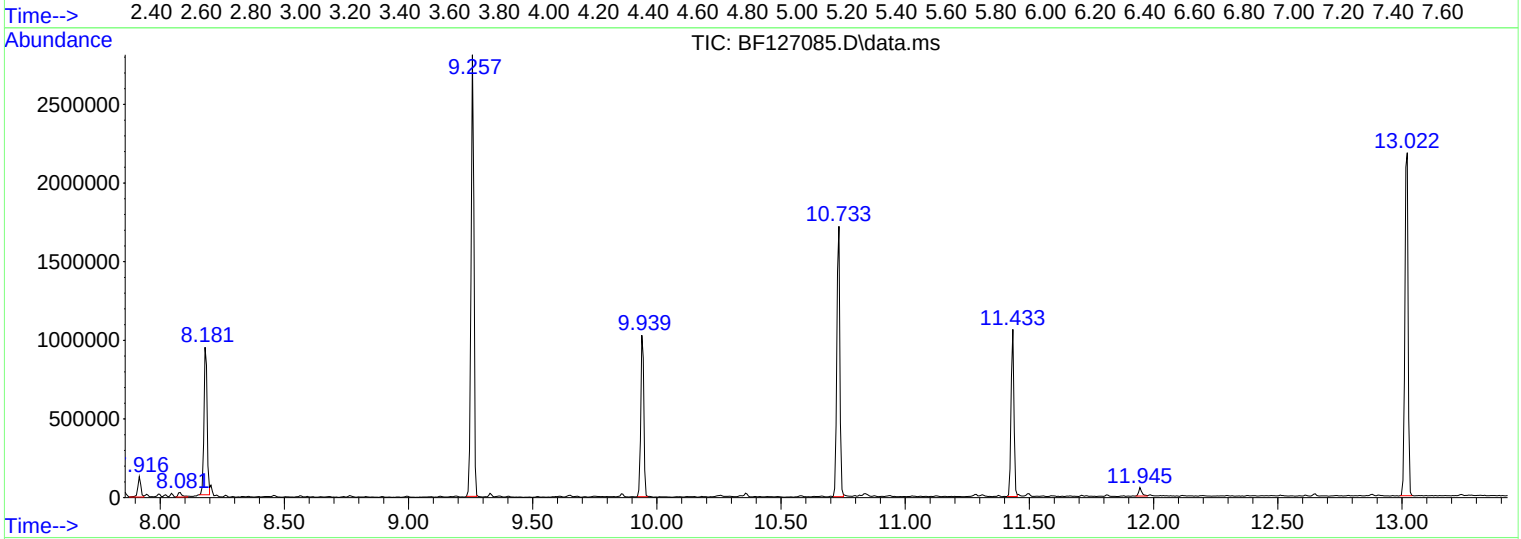
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022522\
Data File : BF127085.D
Acq On : 25 Feb 2022 21:57
Operator : CG\JU
Sample : N1655-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

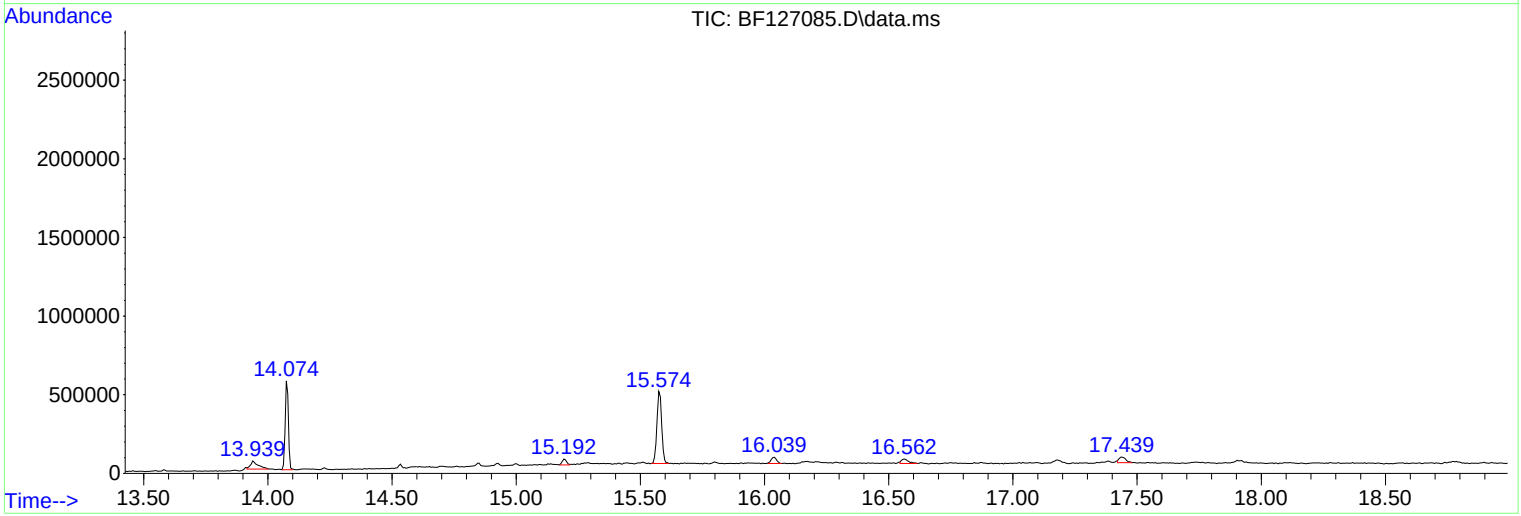
Instrument :
BNA_F
ClientSampleId :
UNK-SOUTH

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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\BF022522\
Data File : BF127085.D
Acq On : 25 Feb 2022 21:57
Operator : CG\JU
Sample : N1655-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UNK-SOUTH

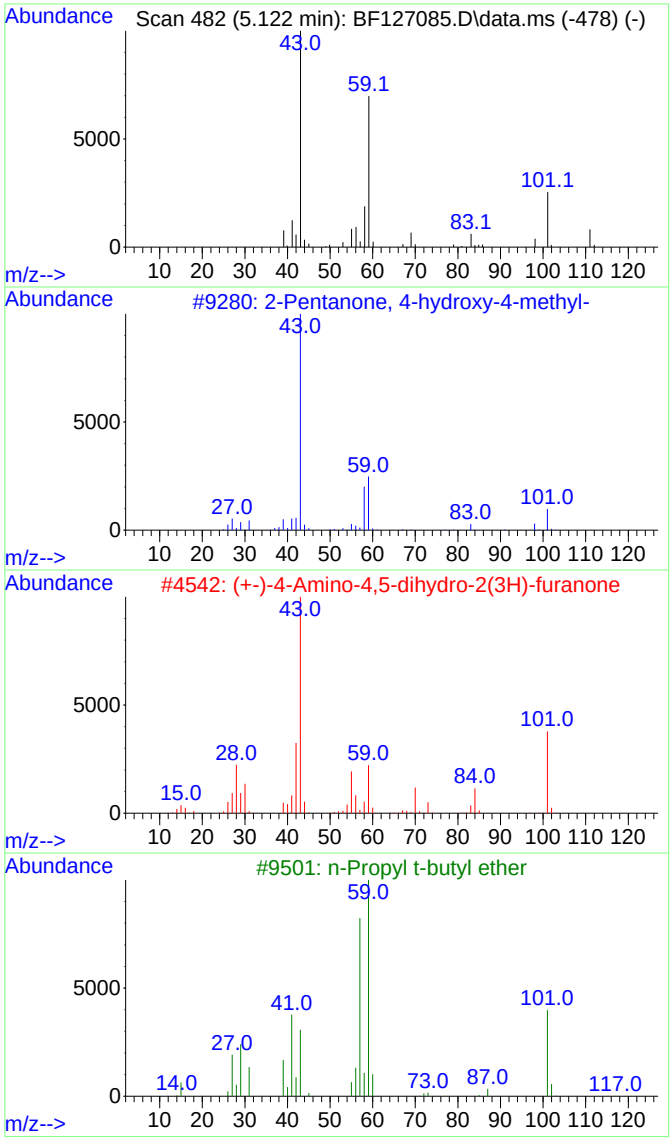
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

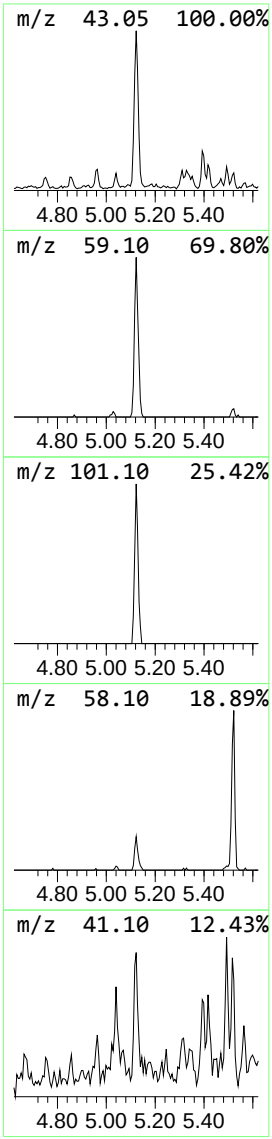
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.122	2.01 ng	62875	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	37
3	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	28
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022522\
Data File : BF127085.D
Acq On : 25 Feb 2022 21:57
Operator : CG\JU
Sample : N1655-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UNK-SOUTH

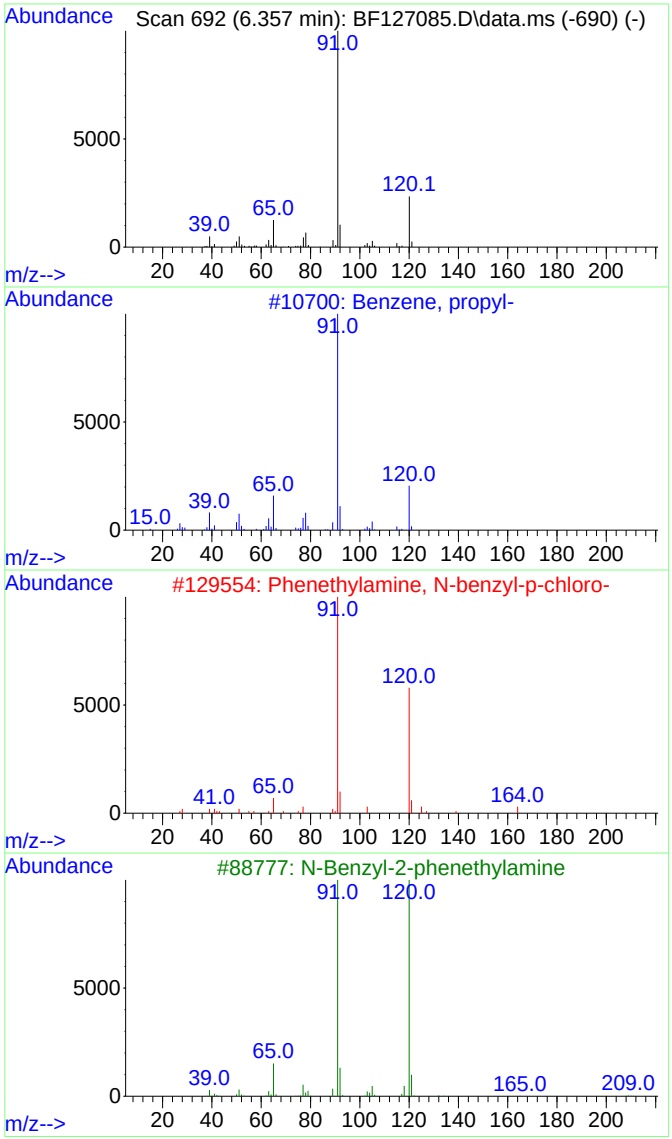
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

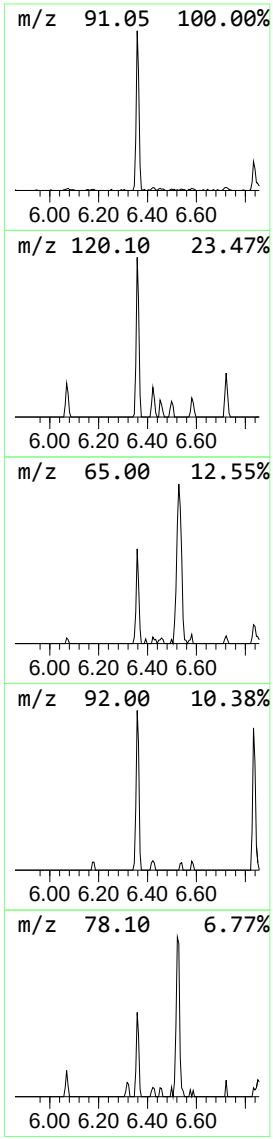
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, propyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.357	2.06 ng	64639	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, propyl-	120	C9H12	000103-65-1	91
2	Phenethylamine, N-benzyl-p-chloro-	245	C15H16ClN	013622-43-0	78
3	N-Benzyl-2-phenethylamine	211	C15H17N	003647-71-0	64
4	Benzeneacetaldehyde	120	C8H8O	000122-78-1	62
5	1-(Benzylamino)propan-2-ol	165	C10H15NO	1000486-84-7	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022522\
Data File : BF127085.D
Acq On : 25 Feb 2022 21:57
Operator : CG\JU
Sample : N1655-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UNK-SOUTH

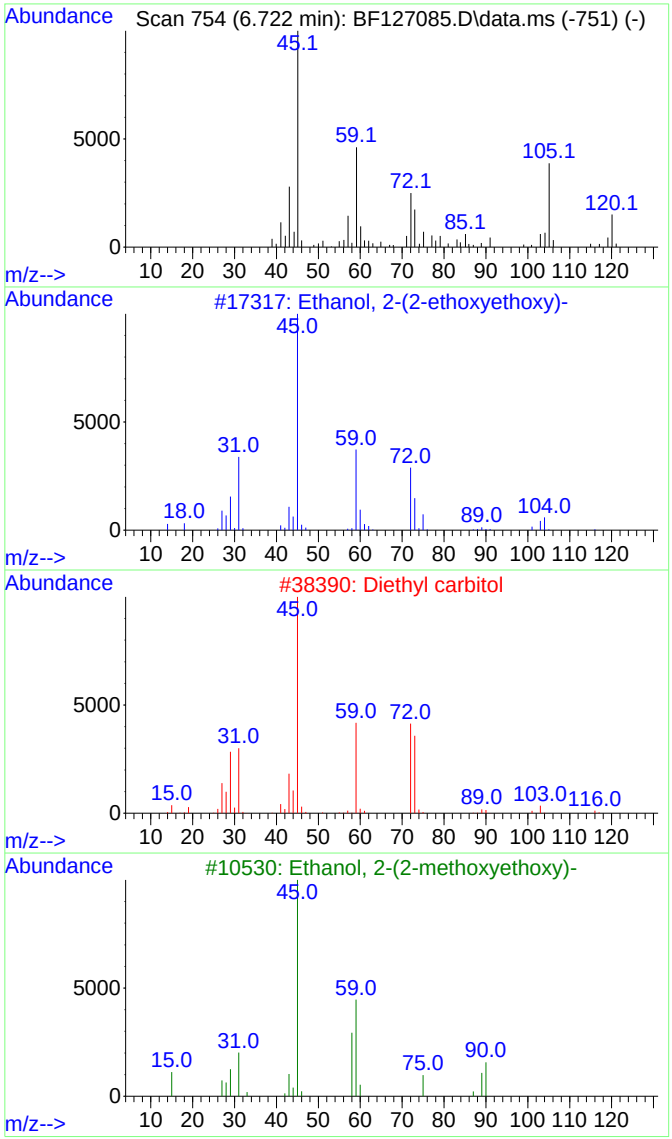
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

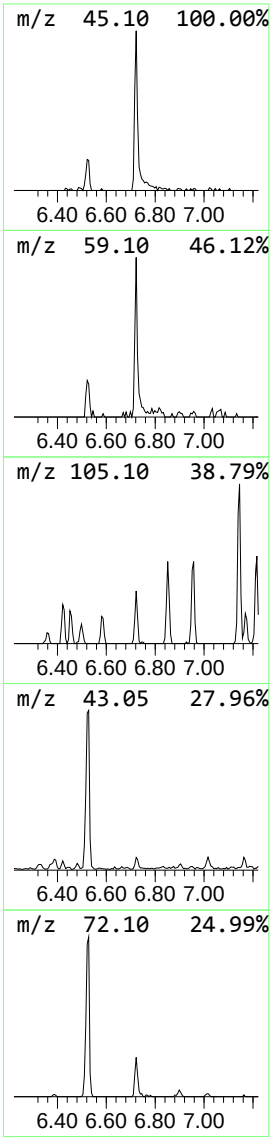
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.722	2.27 ng	71228	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	80
2	Diethyl carbitol	162	C8H18O3	000112-36-7	59
3	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	50
4	Butanoic acid, 4-methoxy-	118	C5H10O3	029006-02-8	42
5	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022522\
Data File : BF127085.D
Acq On : 25 Feb 2022 21:57
Operator : CG\JU
Sample : N1655-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UNK-SOUTH

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

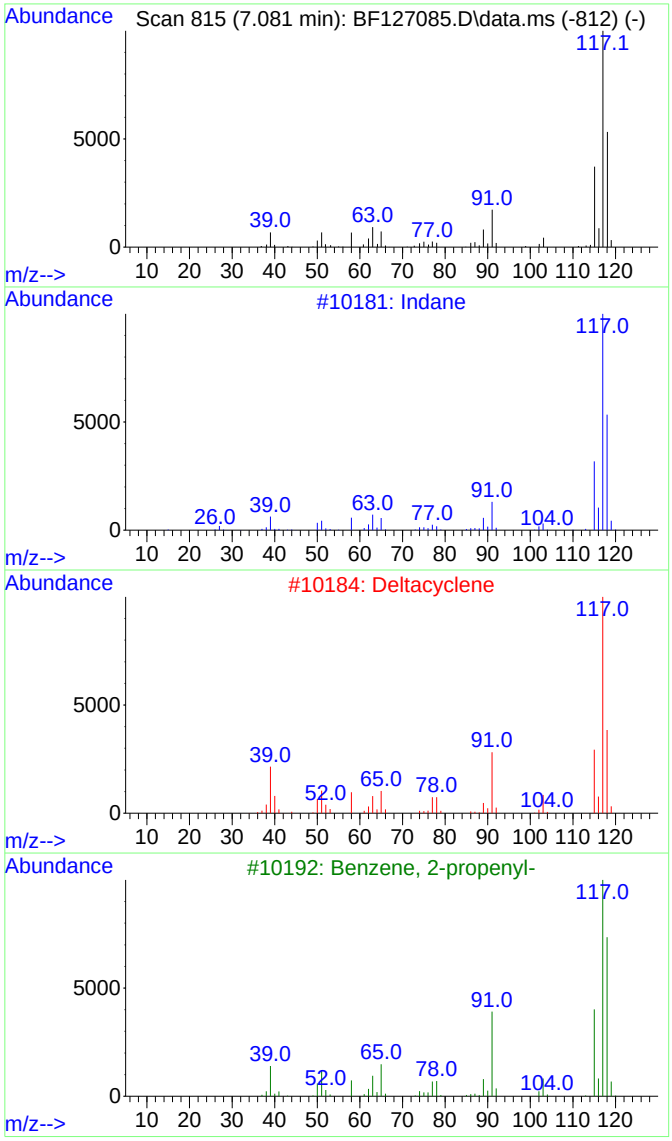
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

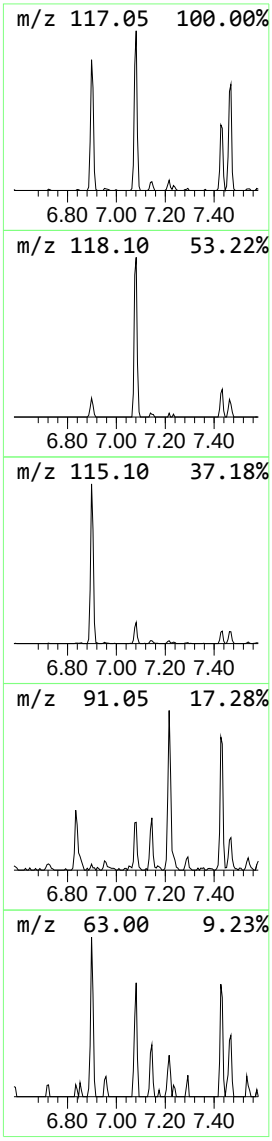
****

Peak Number 5 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.081	2.50 ng	78403	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	87
2	Deltacyclene	118	C9H10	007785-10-6	68
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	64
4	Benzeneethanol, .beta.-ethenyl-	148	C10H12O	006052-63-7	50
5	Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022522\
Data File : BF127085.D
Acq On : 25 Feb 2022 21:57
Operator : CG\JU
Sample : N1655-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UNK-SOUTH

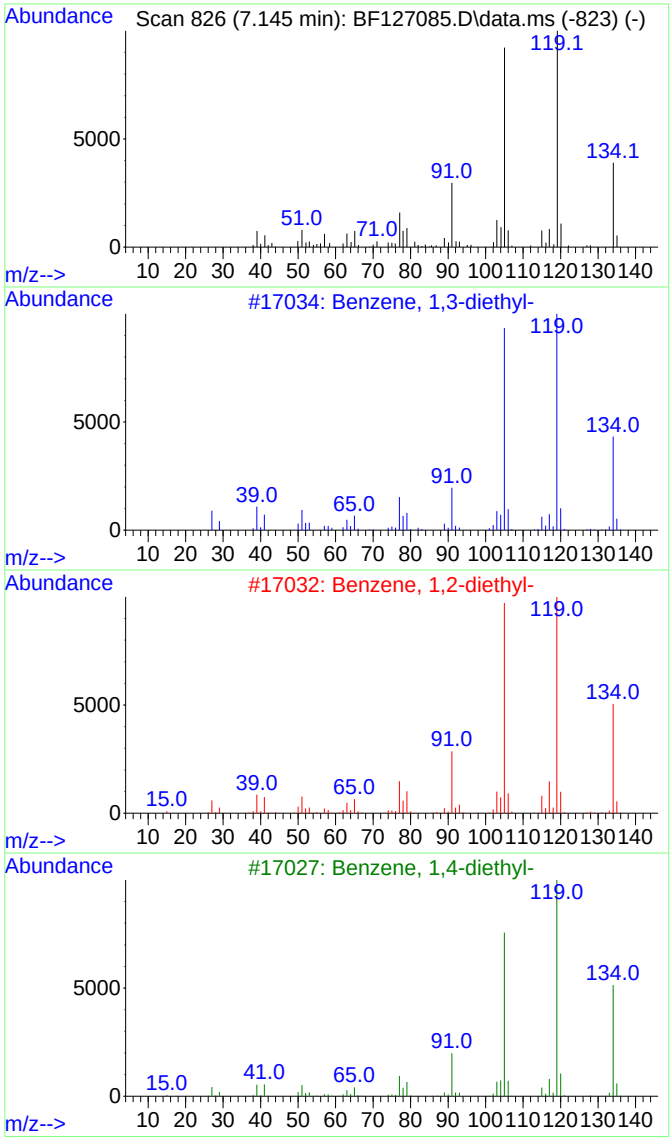
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

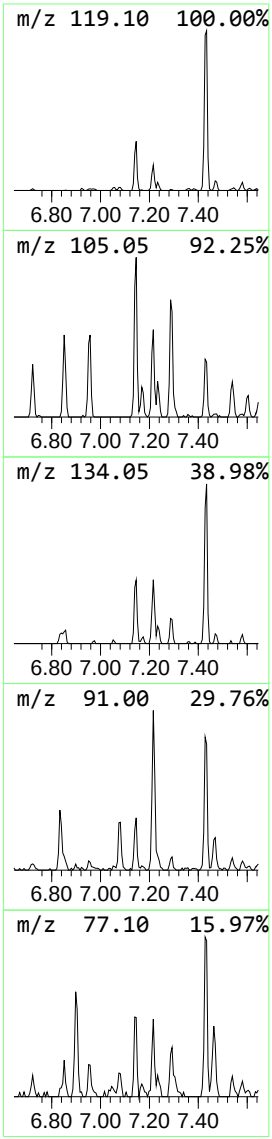
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1,3-diethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.145	2.64 ng	82755	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	97
2	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	94
3	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	91
4	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	91
5	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022522\
Data File : BF127085.D
Acq On : 25 Feb 2022 21:57
Operator : CG\JU
Sample : N1655-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UNK-SOUTH

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

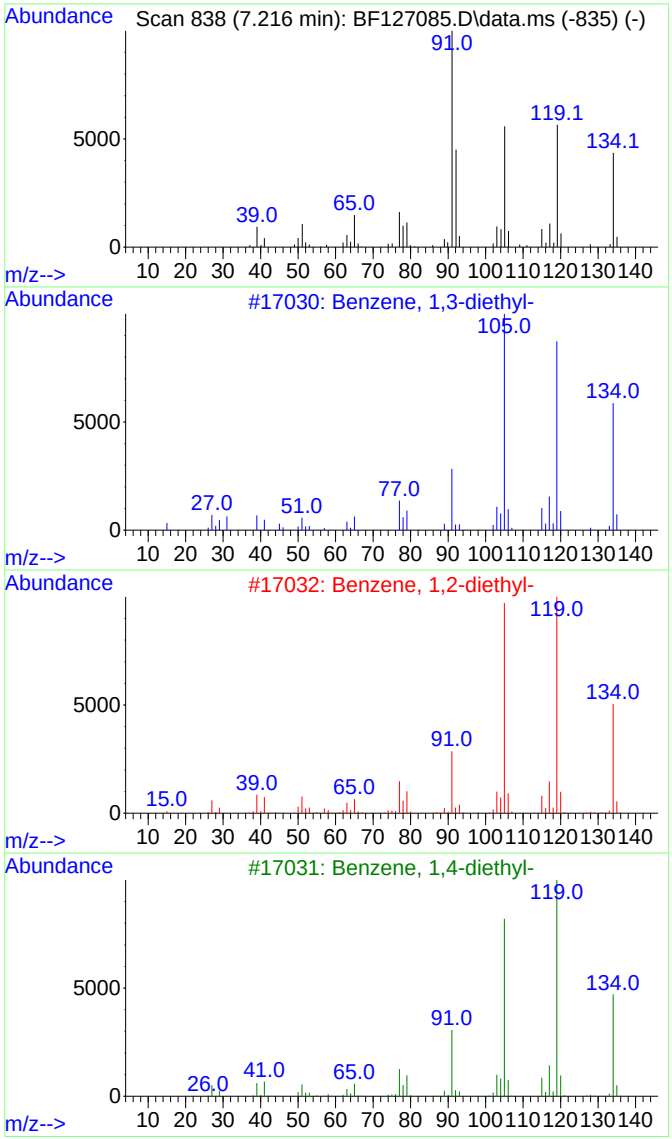
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

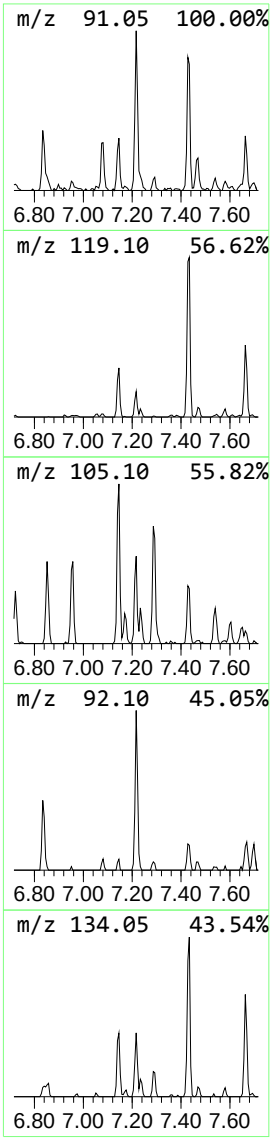
****

Peak Number 7 Benzene, 1,2-diethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.216	2.25 ng	70615	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	93
2	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	92
3	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	92
4	Tetracyclo[3.3.1.1(1,8).0(2,4)]d...	134	C10H14	1000185-58-7	83
5	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022522\
Data File : BF127085.D
Acq On : 25 Feb 2022 21:57
Operator : CG\JU
Sample : N1655-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UNK-SOUTH

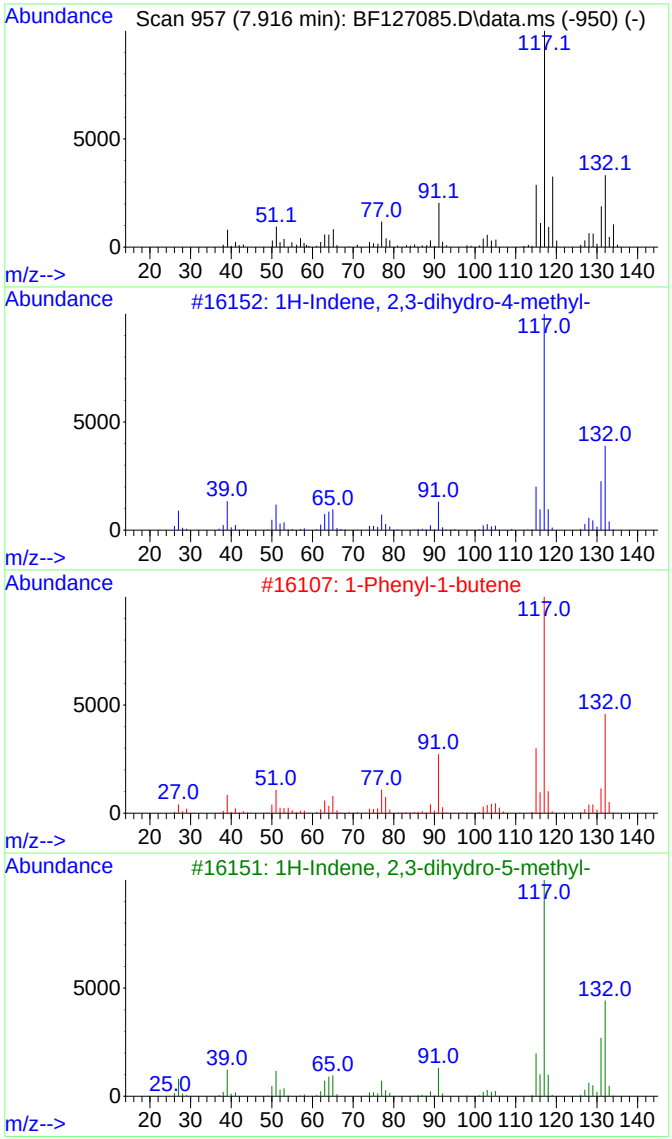
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

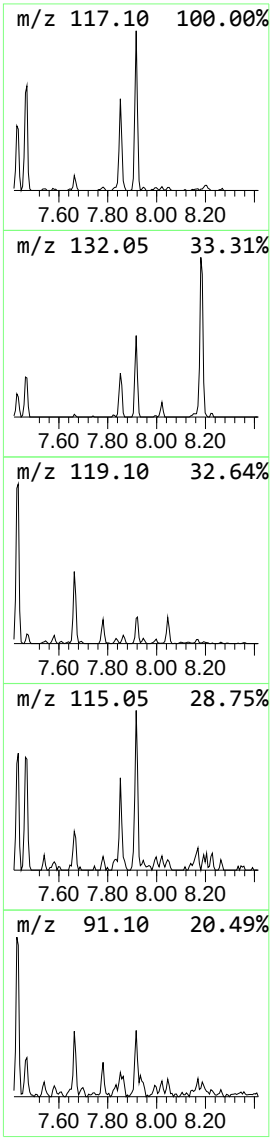
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1H-Indene, 2,3-dihydro-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.916	2.66 ng	110991	Naphthalene-d8	8.181

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	93
2	1-Phenyl-1-butene	132	C10H12	000824-90-8	93
3	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	89
4	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87
5	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022522\
Data File : BF127085.D
Acq On : 25 Feb 2022 21:57
Operator : CG\JU
Sample : N1655-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UNK-SOUTH

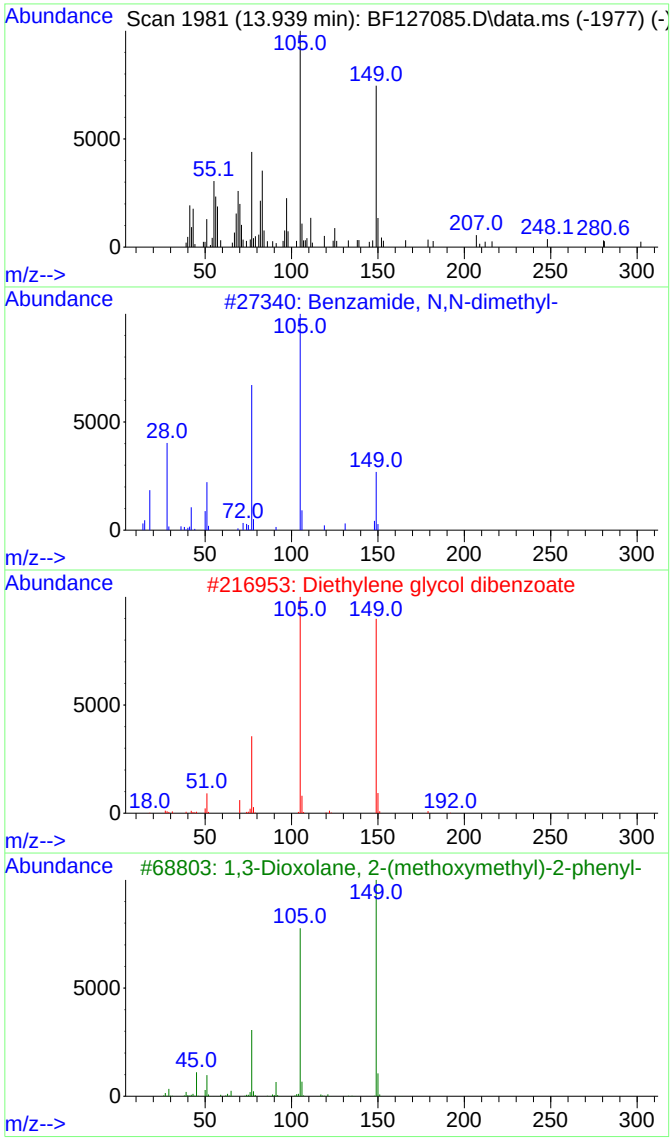
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

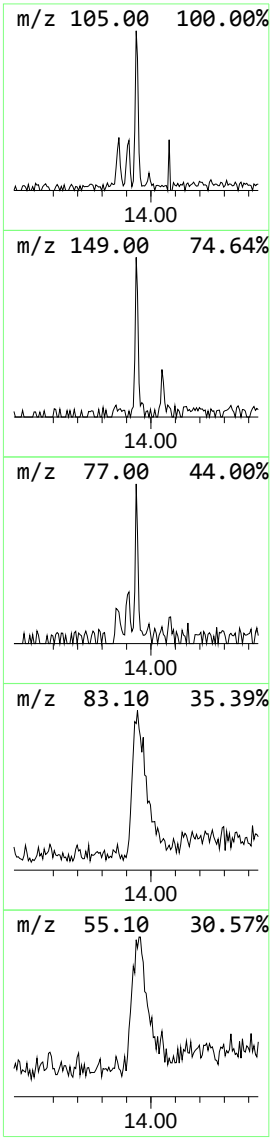
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzamide, N,N-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.939	4.27 ng	109126	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N,N-dimethyl-	149	C9H11NO	000611-74-5	52
2	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	50
3	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	50
4	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	50
5	Phthalic acid, isobutyl 2-(2-met...	364	C21H32O5	1000314-93-8	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022522\
Data File : BF127085.D
Acq On : 25 Feb 2022 21:57
Operator : CG\JU
Sample : N1655-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UNK-SOUTH

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

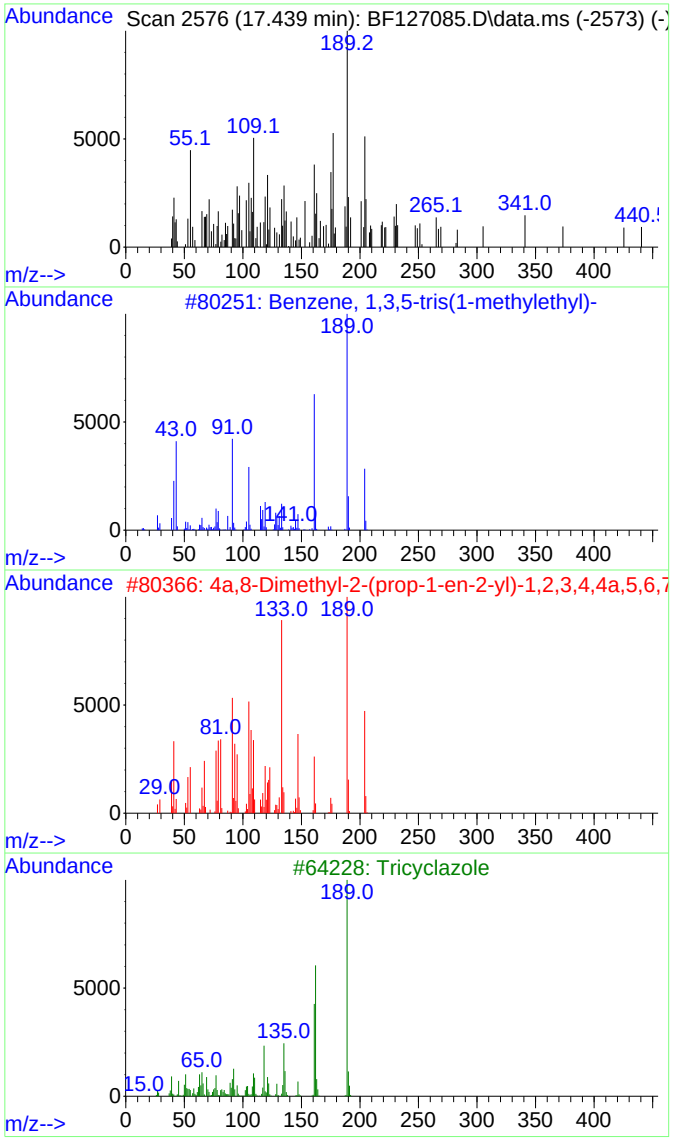
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

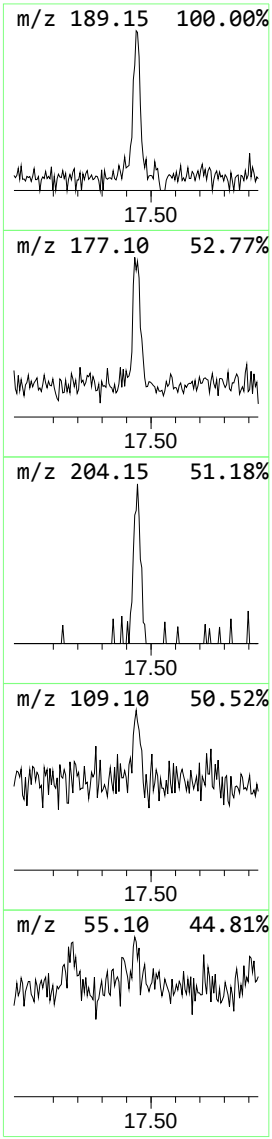
****

Peak Number 10 unknown17.439 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.439	2.21 ng	66225	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3,5-tris(1-methylethyl)-	204	C15H24	000717-74-8	46
2	4a,8-Dimethyl-2-(prop-1-en-2-yl)...	204	C15H24	103827-22-1	43
3	Tricyclazole	189	C9H7N3S	041814-78-2	38
4	(3S,6aR,6bR,8aR,14bR)-3-methoxy-...	440	C31H52O	1000441-97-8	38
5	1R,4S,7S,11R-2,2,4,8-Tetramethyl...	204	C15H24	1208118-28-8	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022522\
Data File : BF127085.D
Acq On : 25 Feb 2022 21:57
Operator : CG\JU
Sample : N1655-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UNK-SOUTH

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-...	5.122	2.0	ng	62875	1	6.898	626783	20.0
Benzene, propyl-	6.357	2.1	ng	64639	1	6.898	626783	20.0
Ethanol, 2-(2-e...	6.722	2.3	ng	71228	1	6.898	626783	20.0
Indane	7.081	2.5	ng	78403	1	6.898	626783	20.0
Benzene, 1,3-di...	7.145	2.6	ng	82755	1	6.898	626783	20.0
Benzene, 1,2-di...	7.216	2.3	ng	70615	1	6.898	626783	20.0
1H-Indene, 2,3-...	7.916	2.7	ng	110991	2	8.181	835964	20.0
Benzamide, N,N-...	13.939	4.3	ng	109126	5	14.074	511491	20.0
unknown17.439	17.439	2.2	ng	66225	6	15.574	600290	20.0