LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008262.D
Acq On : 07 Dec 2021 21:47
Operator : CG/JU
Sample : M4949-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
VNJ-221

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_P\Methods\8270E-BP112521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008262.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.917	322	328	338	rVB	24516	37836	1.12%	0.188%
2	5.375	400	406	416	rBV	1229144	1803656	53.47%	8.967%
3	6.969	670	677	699	rBV	1076292	1837895	54.49%	9.138%
4	7.781	808	815	824	rBV	231833	359846	10.67%	1.789%
5	8.946	999	1013	1028	rBV	668492	1175937	34.86%	5.847%
6	10.387	1253	1258	1270	rBV2	18703	48972	1.45%	0.243%
7	10.581	1284	1291	1305	rBV	253218	451347	13.38%	2.244%
8	13.051	1704	1711	1725	rBV	1631514	2321740	68.83%	11.543%
9	14.098	1882	1889	1896	rBV3	17944	37797	1.12%	0.188%
10	14.334	1920	1929	1936	rBV5	13101	37999	1.13%	0.189%
11	14.434	1939	1946	1953	rBV	358584	547686	16.24%	2.723%
12	15.240	2079	2083	2090	rBV2	16629	36050	1.07%	0.179%
13	15.934	2194	2201	2209	rBV	1203754	1800875	53.39%	8.954%
14	17.122	2398	2403	2409	rVB2	32127	44200	1.31%	0.220%
15	17.198	2409	2416	2421	rBV	430278	673693	19.97%	3.349%
16	17.239	2421	2423	2429	rVB	34651	44640	1.32%	0.222%
17	17.322	2434	2437	2445	rVB5	22529	39989	1.19%	0.199%
18	17.492	2462	2466	2477	rBV3	12876	33993	1.01%	0.169%
19	18.098	2564	2569	2577	rBV3	63747	99254	2.94%	0.493%
20	19.216	2755	2759	2766	rBV	111064	160614	4.76%	0.799%
21	19.569	2816	2819	2829	rVB	78874	117489	3.48%	0.584%
22	19.769	2847	2853	2866	rBV	2848342	3373041	100.00%	16.770%
23	20.445	2966	2968	2974	rVB	36938	43405	1.29%	0.216%
24	20.975	3053	3058	3062	rBV	207623	359116	10.65%	1.785%
25	21.027	3062	3067	3072	rVV	375999	608199	18.03%	3.024%
26	21.080	3072	3076	3083	rVV	1110448	1402459	41.58%	6.973%
27	21.145	3085	3087	3095	rVV	73439	118028	3.50%	0.587%
28	21.216	3096	3099	3104	rVB	160412	168576	5.00%	0.838%
29	21.304	3108	3114	3118	rVV	718561	1024553	30.37%	5.094%
30	21.339	3118	3120	3125	rVB	99414	112759	3.34%	0.561%
31	22.969	3393	3397	3401	rBV2	112989	187703	5.56%	0.933%
32	23.698	3515	3521	3529	rVB2	491671	1004072	29.77%	4.992%

Sum of corrected areas: 20113419

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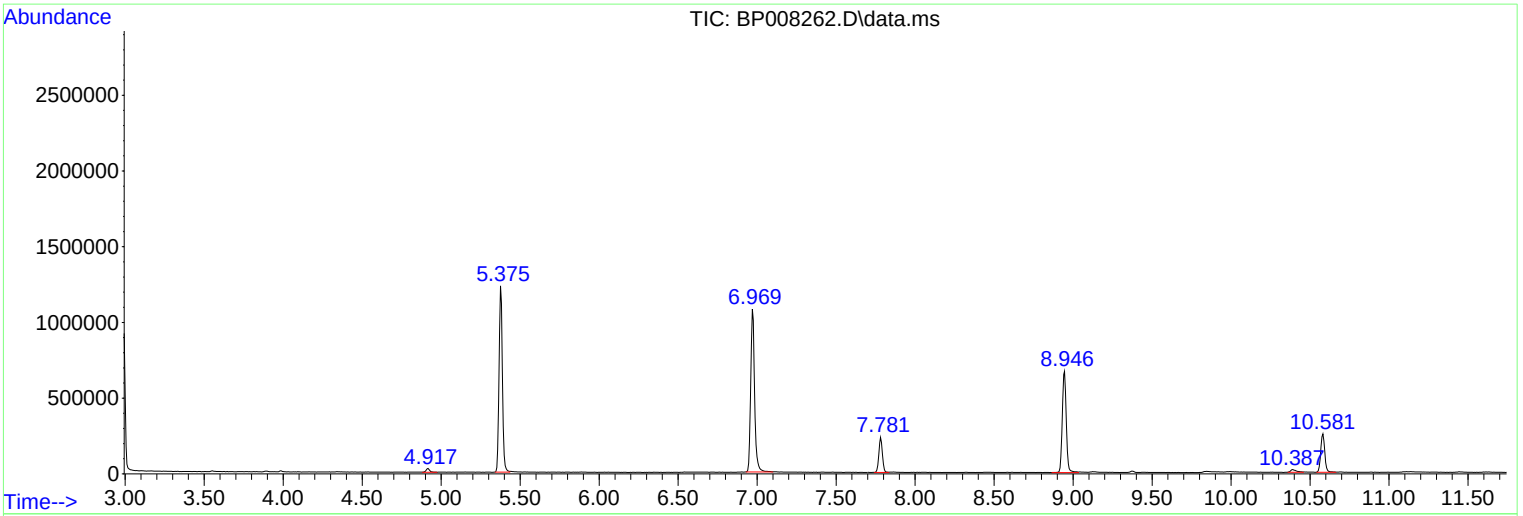
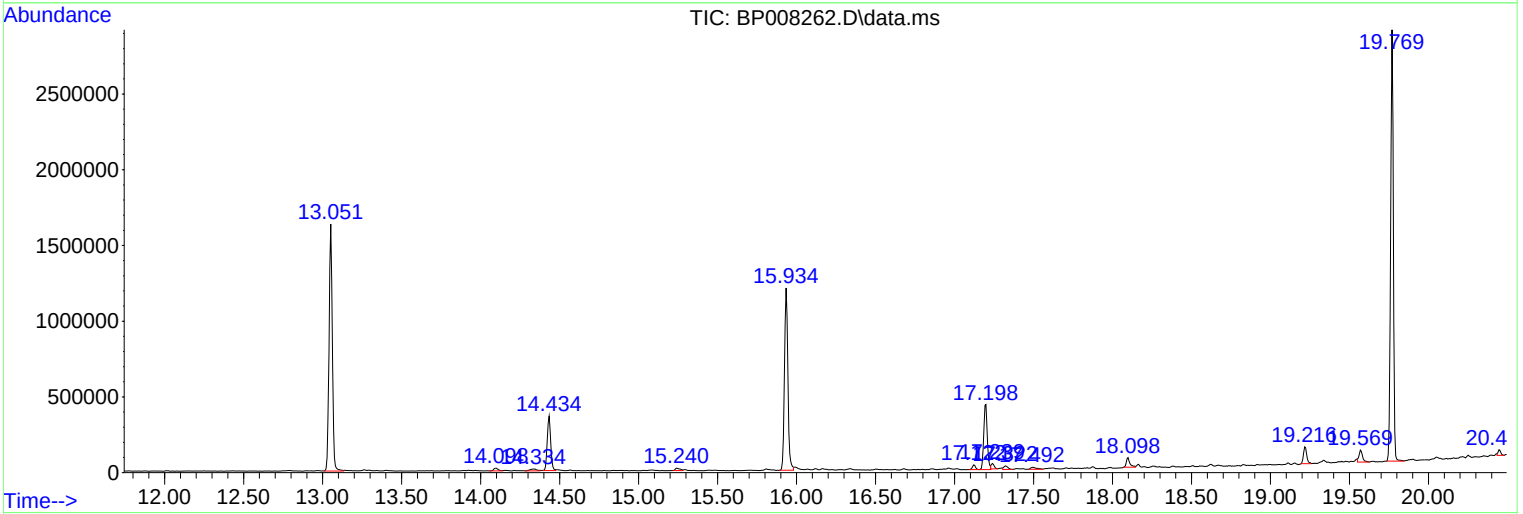
Sample : M4949-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

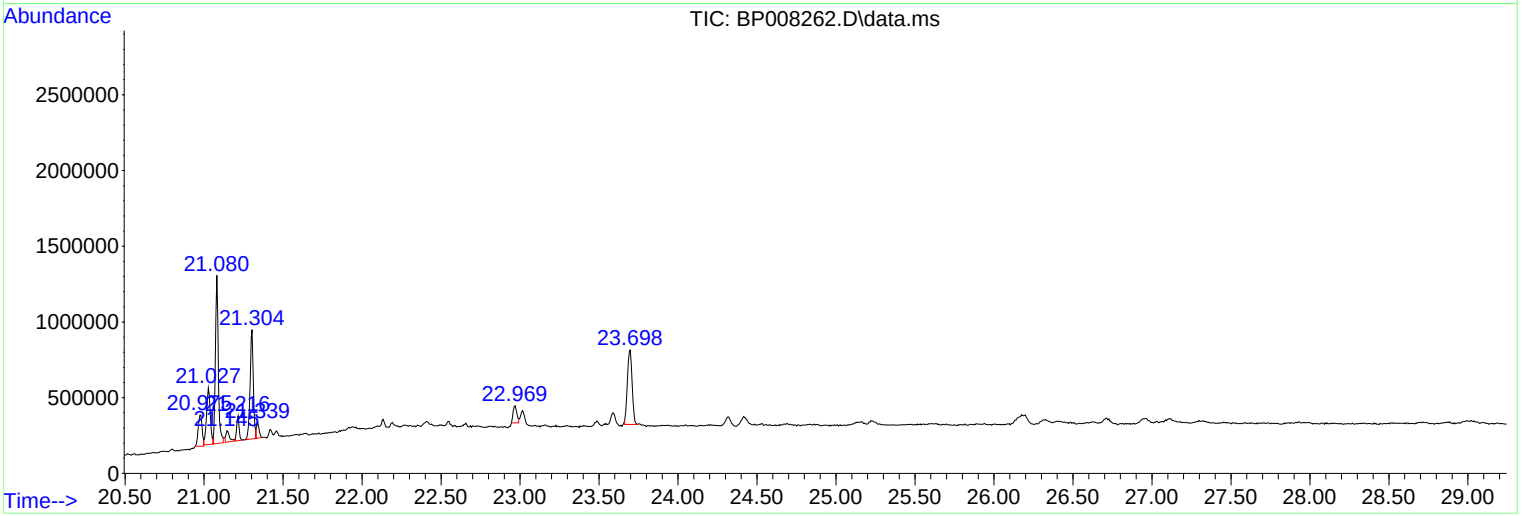
Instrument :
BNA_P
ClientSampleId :
VNJ-221

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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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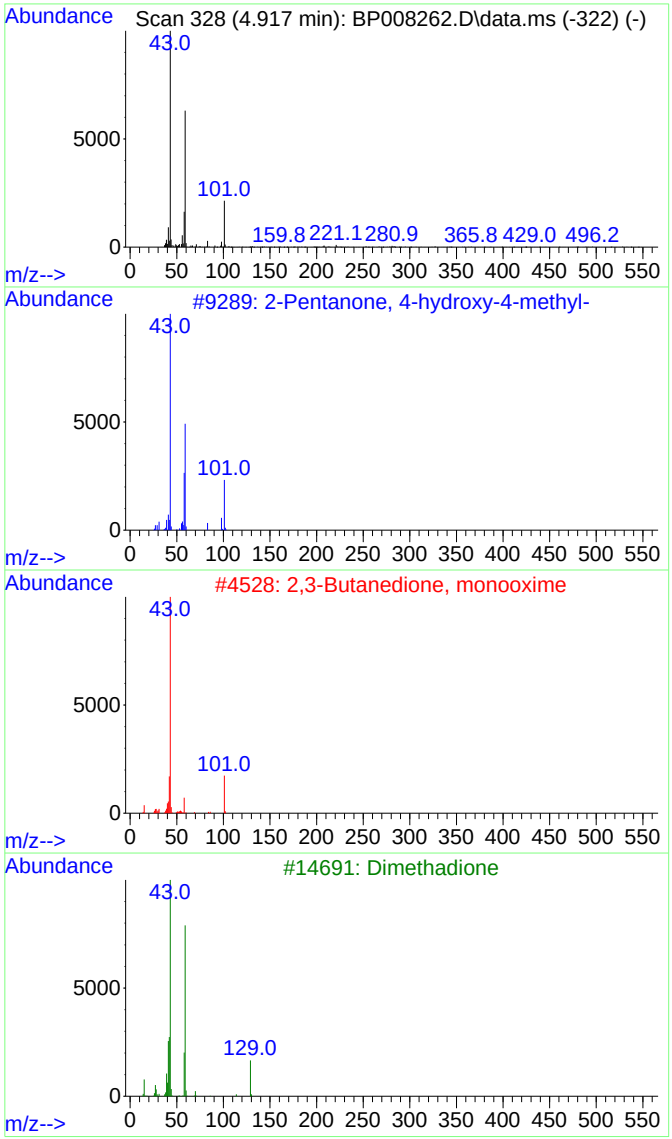
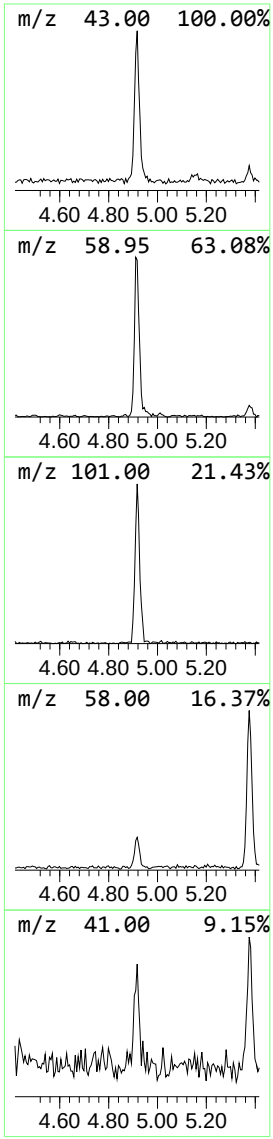
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.917	2.10 ng	37836	1,4-Dichlorobenzene-d4	7.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
3	Dimethadione	129	C5H7NO3	000695-53-4	33
4	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
5	3-Octanol	130	C8H18O	000589-98-0	25





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ClientSampleId :
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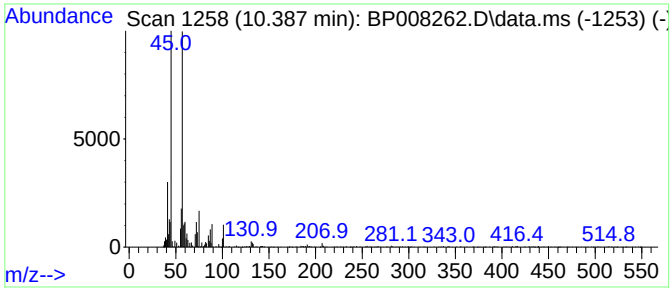
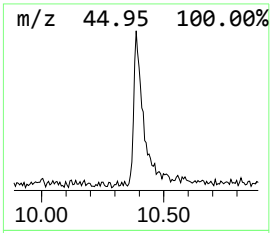
****

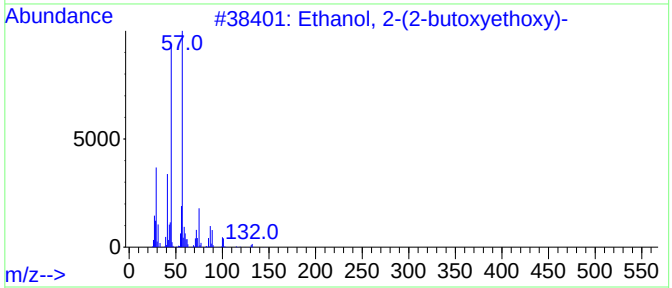
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

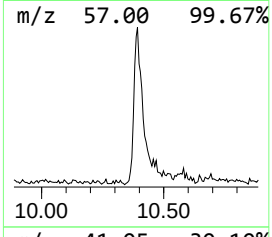
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.387	2.17 ng	48972	Naphthalene-d8	10.581

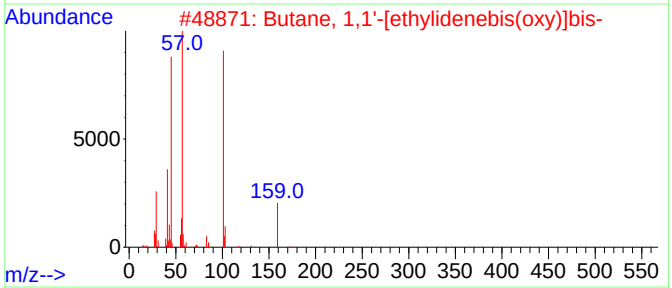
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	80
2	Butane, 1,1'-[ethylidenebis(oxy)...	174	C10H22O2	000871-22-7	50
3	Pentaethylene glycol	238	C10H22O6	004792-15-8	47
4	Pentaethylene glycol monododecyl...	406	C22H46O6	003055-95-6	47
5	Triethylene glycol	150	C6H14O4	000112-27-6	47

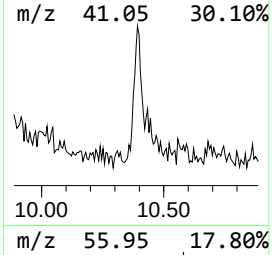


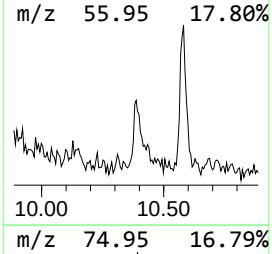


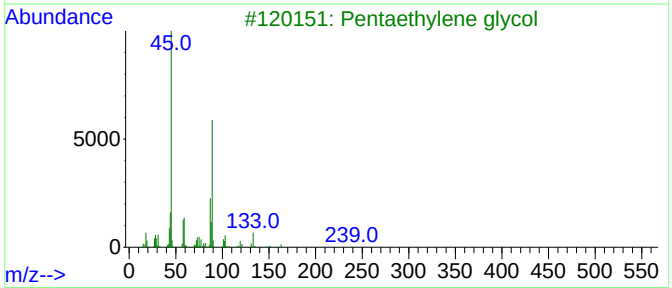


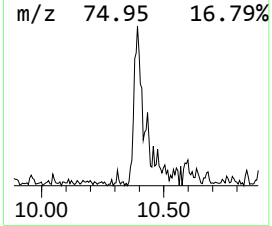












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
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Acq On : 07 Dec 2021 21:47
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Sample : M4949-01
Misc :
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Instrument :
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ClientSampleId :
VNJ-221

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

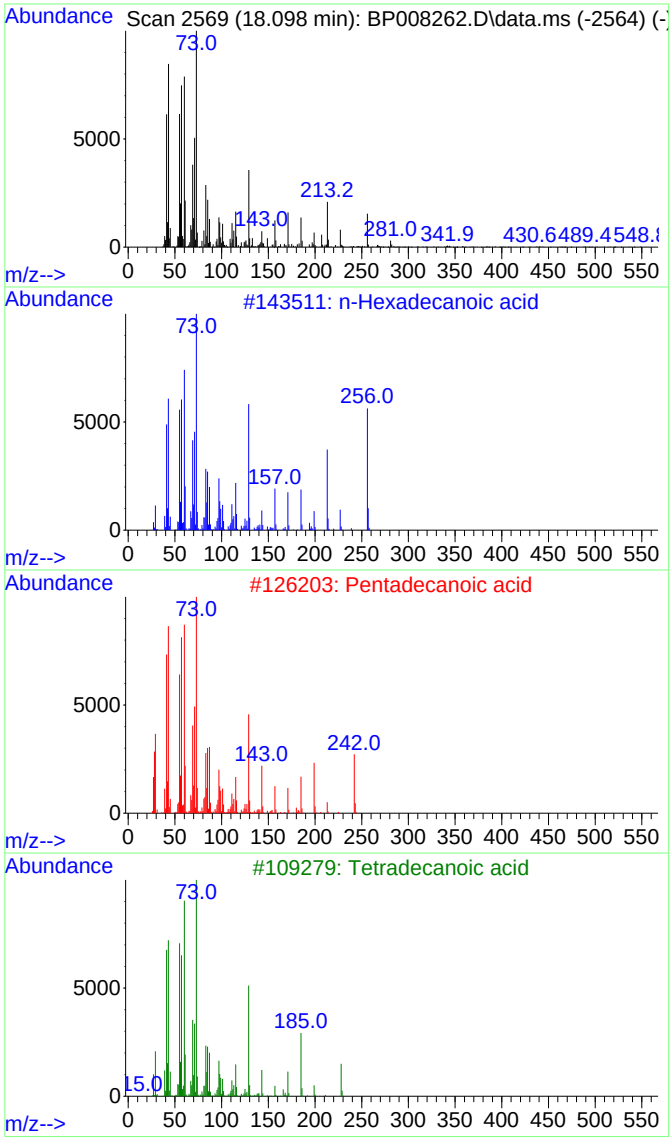
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

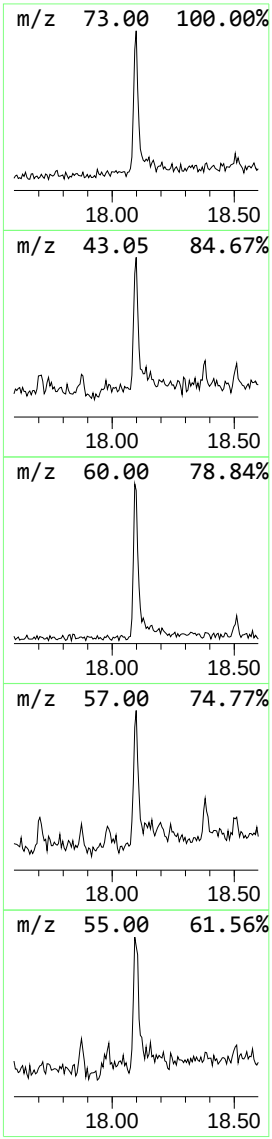
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.098	2.95 ng	99254	Phenanthrene-d10	17.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4	Dodecanoic acid	200	C12H24O2	000143-07-7	62
5	Tridecanoic acid	214	C13H26O2	000638-53-9	58





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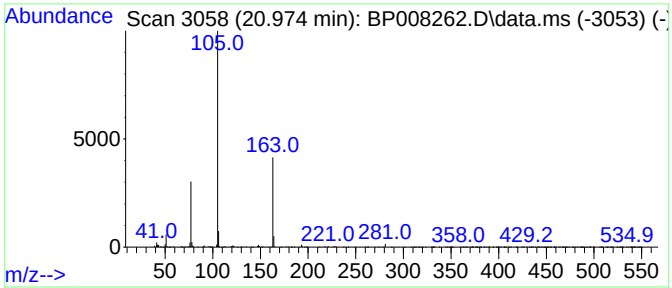
TIC Integration Parameters: LSCINT.P

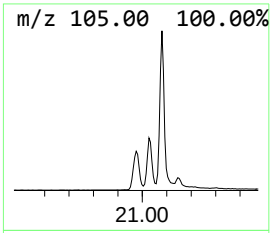
****

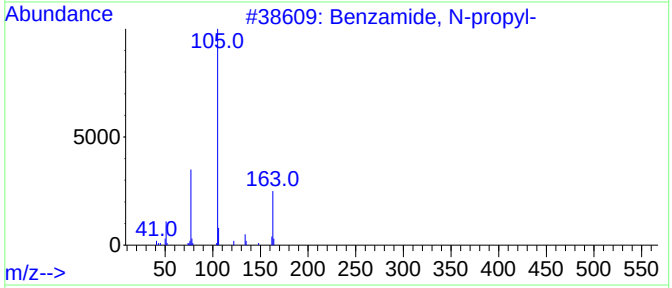
Peak Number 5 Benzamide, N-propyl- Concentration Rank 3

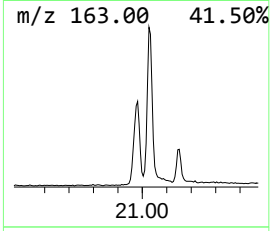
R.T.	EstConc	Area	Relative to ISTD	R.T.
20.974	7.01 ng	359116	Chrysene-d12	21.304

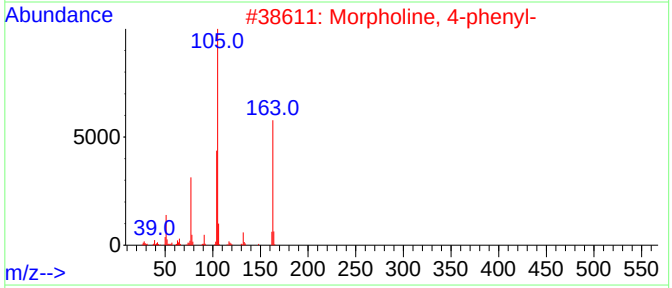
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-propyl-	163	C10H13NO	010546-70-0	72
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	72
3	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	50
4	1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	40
5	Oxazol-5(4H)-one, 4-(3,5-dibromo...	421	C16H9Br2NO3	113425-80-2	27

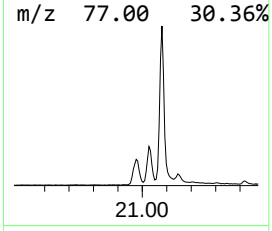


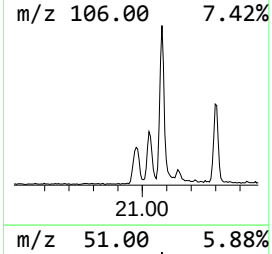


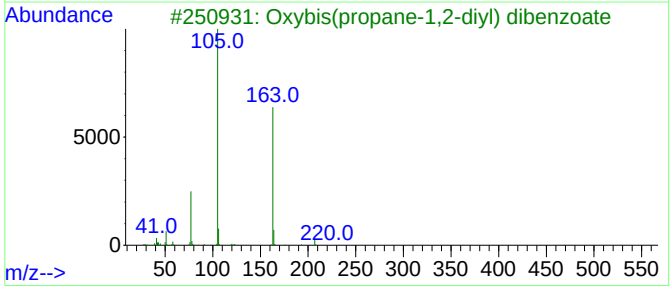


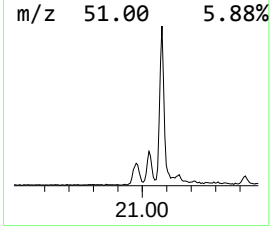












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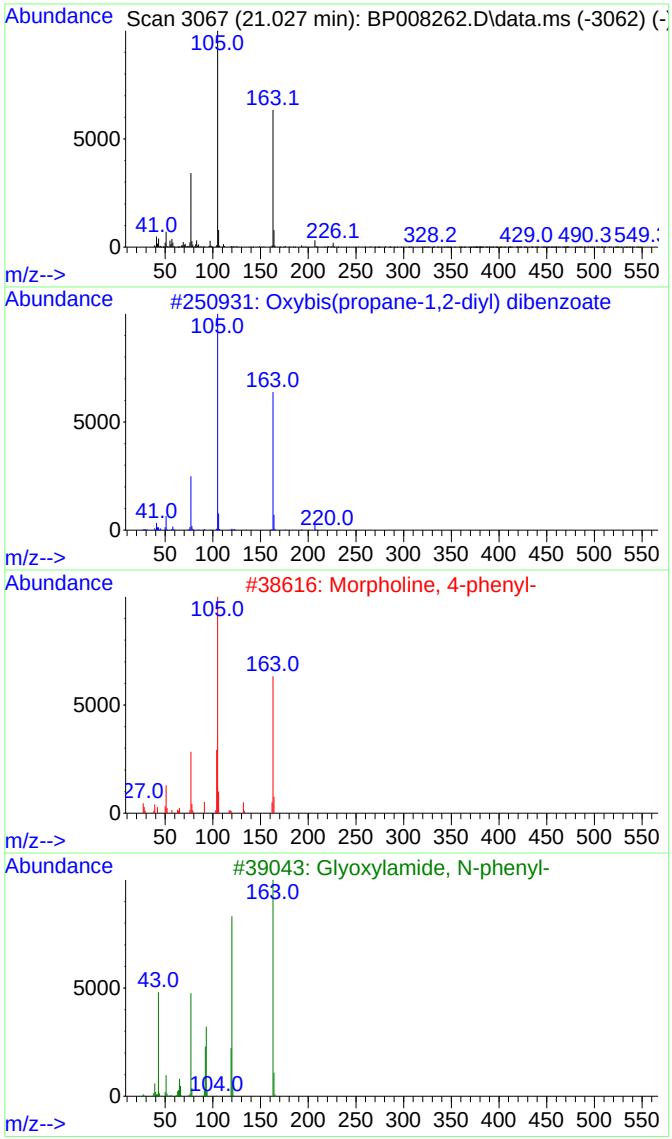
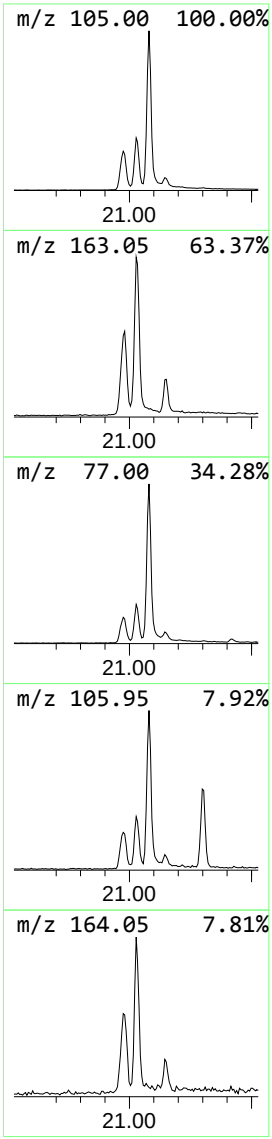
****

Peak Number 6 Oxybis(propane-1,2-diyl) di... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.027	11.87 ng	608199	Chrysene-d12	21.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	87
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	72
3	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	47
4	Decyl methyl phthalate	320	C19H28O4	256481-38-6	43
5	Benzoic acid, 2-benzyloxy-3-brom...	348	C17H17BrO3	1000191-33-3	40





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TIC Library : C:\Database\NIST20.L
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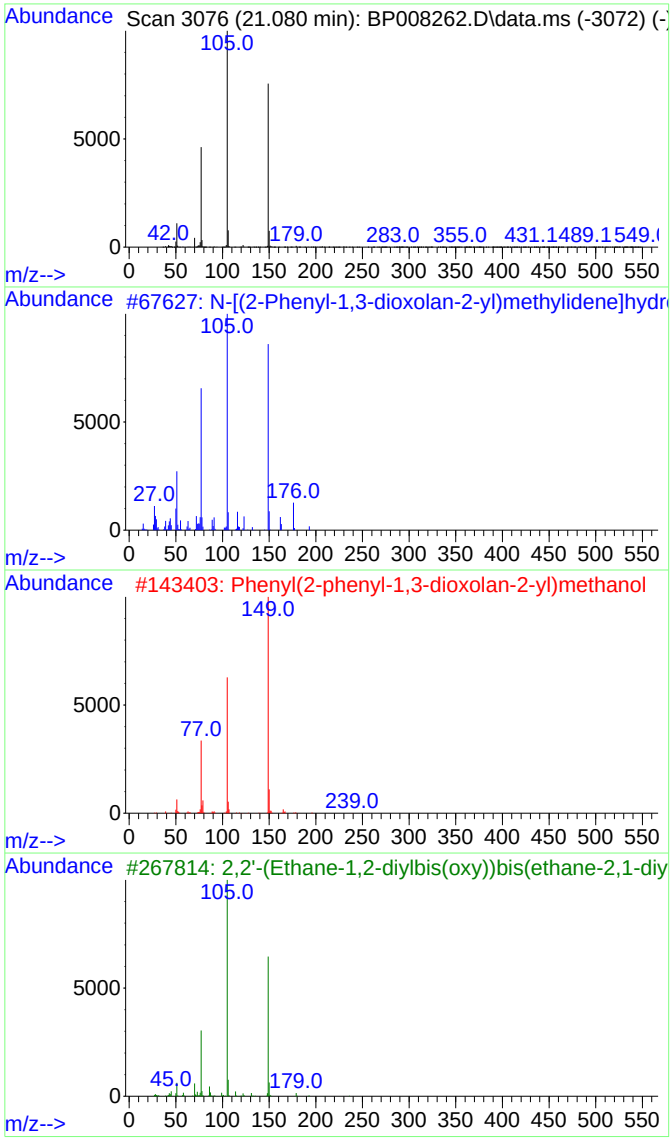
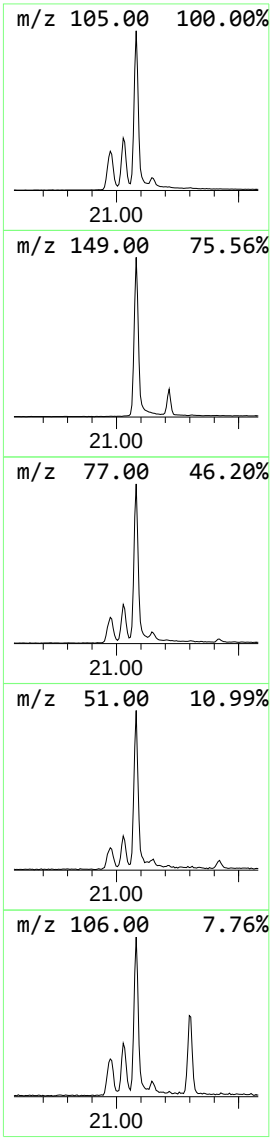
****
Peak Number 7 N-[(2-Phenyl-1,3-dioxolan-2... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.080	27.38 ng	1402460	Chrysene-d12	21.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-[(2-Phenyl-1,3-dioxolan-2-yl)m...	193	C10H11NO3	1000411-48-9	78
2	Phenyl(2-phenyl-1,3-dioxolan-2-y...	256	C16H16O3	005694-69-9	78
3	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	74
4	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	74
5	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008262.D
Acq On : 07 Dec 2021 21:47
Operator : CG/JU
Sample : M4949-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
VNJ-221

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

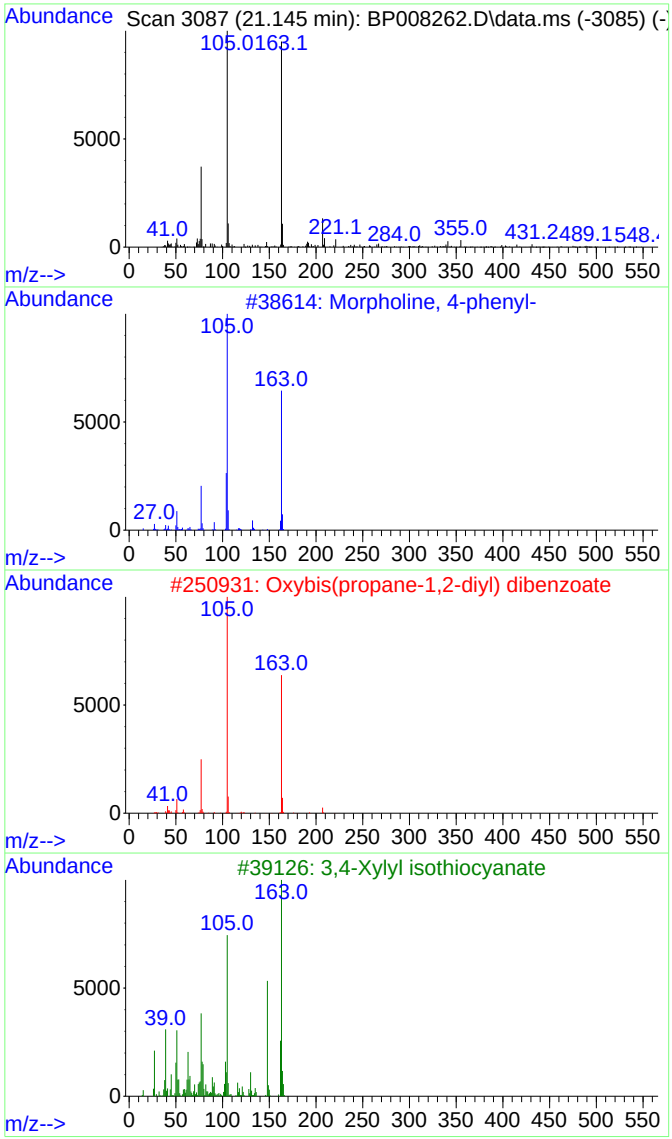
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

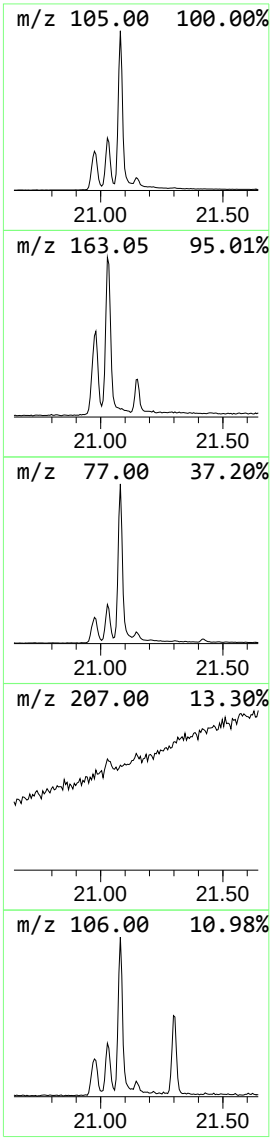
****

Peak Number 8 Morpholine, 4-phenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.145	2.30 ng	118028	Chrysene-d12	21.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	72
2	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	64
3	3,4-Xylyl isothiocyanate	163	C9H9NS	019241-17-9	64
4	N-(4-Formyl-phenyl)-N-methyl-for...	163	C9H9NO2	079213-80-2	50
5	Phthalic acid, 3,4-dimethylpheny...	284	C17H16O4	1000315-69-7	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008262.D
Acq On : 07 Dec 2021 21:47
Operator : CG/JU
Sample : M4949-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
VNJ-221

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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-...	4.917	2.1	ng	37836	1	7.781	359846	20.0
Ethanol, 2-(2-b...	10.387	2.2	ng	48972	2	10.581	451347	20.0
n-Hexadecanoic ...	18.098	3.0	ng	99254	4	17.198	673693	20.0
Benzamide, N-pr...	20.974	7.0	ng	359116	5	21.304	1024550	20.0
Oxybis(propane-...	21.027	11.9	ng	608199	5	21.304	1024550	20.0
N-[(2-Phenyl-1,...	21.080	27.4	ng	1402460	5	21.304	1024550	20.0
Morpholine, 4-p...	21.145	2.3	ng	118028	5	21.304	1024550	20.0