LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011321\
Data File : BP004539.D
Acq On : 13 Jan 2021 16:04
Operator : CG/JU
Sample : M1073-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : VNJ-217

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-BP011221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP004539.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.399	370	376	389	rBV	2085897	3194194	39.28%	7.348%
2	6.981	636	645	664	rBV	1897561	3261110	40.10%	7.502%
3	7.810	778	786	794	rBV	719246	1139666	14.01%	2.622%
4	8.969	974	983	1002	rBV	1224166	2079137	25.57%	4.783%
5	10.604	1251	1261	1277	rBV	898467	1576894	19.39%	3.627%
6	13.075	1674	1681	1700	rBV	3591403	5406838	66.49%	12.437%
7	13.910	1816	1823	1828	rBV	52828	84800	1.04%	0.195%
8	14.457	1906	1916	1929	rBV	1354558	2164530	26.62%	4.979%
9	15.957	2164	2171	2188	rBV	2845766	4257407	52.35%	9.793%
10	17.222	2379	2386	2392	rBV	1749407	2543228	31.27%	5.850%
11	18.110	2532	2537	2546	rBV2	61749	133869	1.65%	0.308%
12	18.851	2658	2663	2668	rBV	331632	405280	4.98%	0.932%
13	18.933	2674	2677	2682	rBV	89982	114552	1.41%	0.264%
14	19.239	2724	2729	2735	rBV	136989	189155	2.33%	0.435%
15	19.469	2764	2768	2771	rBV	76495	97854	1.20%	0.225%
16	19.592	2786	2789	2798	rVB	113999	176196	2.17%	0.405%
17	19.786	2816	2822	2834	rBV	6670915	8131896	100.00%	18.706%
18	20.451	2933	2935	2941	rVB	68317	83332	1.02%	0.192%
19	20.657	2966	2970	2975	rBV	203679	233666	2.87%	0.538%
20	21.027	3029	3033	3040	rBV2	346611	605815	7.45%	1.394%
21	21.092	3040	3044	3050	rVB	280817	372010	4.57%	0.856%
22	21.316	3077	3082	3087	rBV	2685582	3390220	41.69%	7.799%
23	21.427	3098	3101	3105	rBV	70721	90183	1.11%	0.207%
24	23.668	3475	3482	3498	rVB2	1871269	3740341	46.00%	8.604%

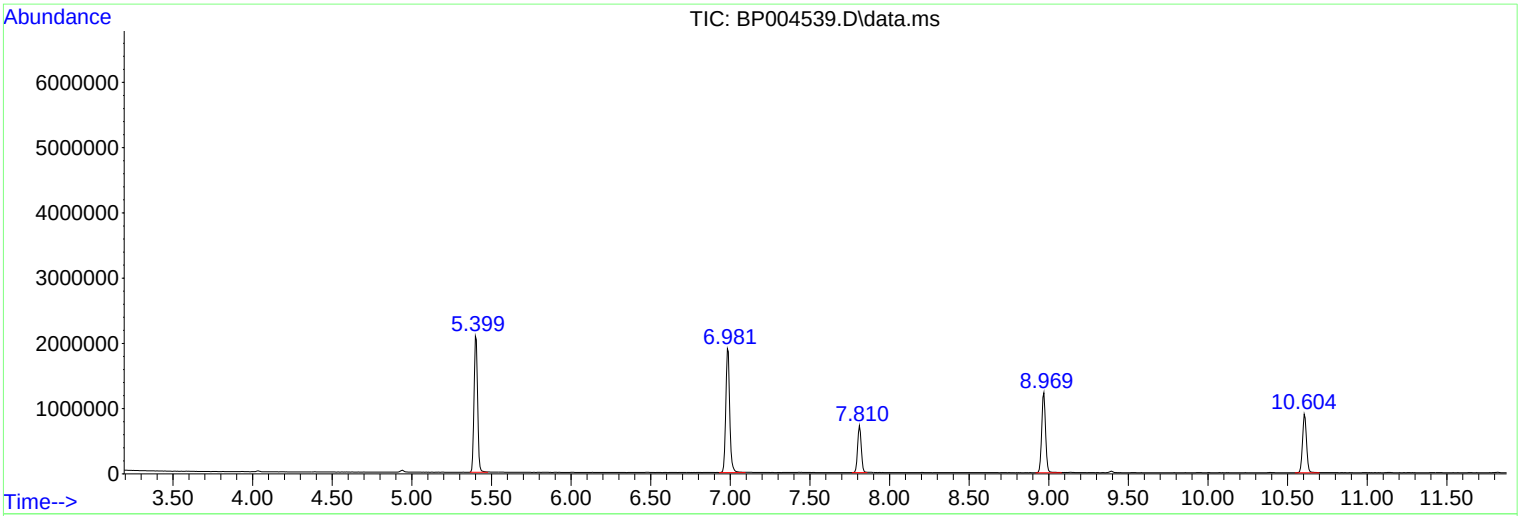
Sum of corrected areas: 43472173

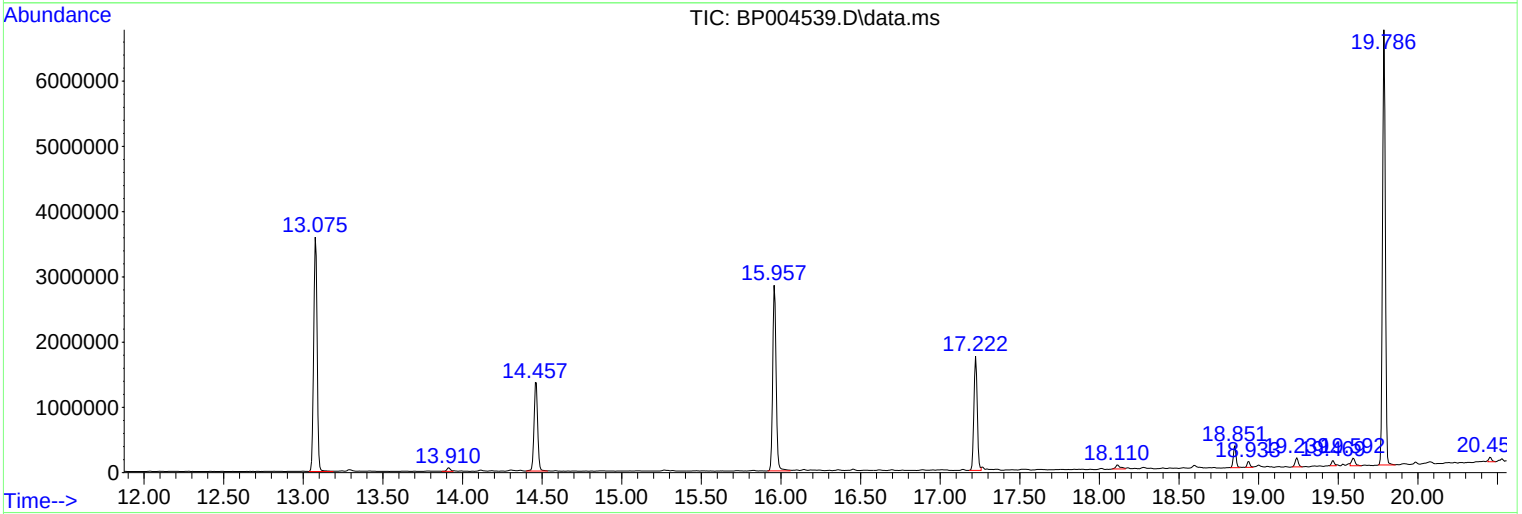
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011321\
Data File : BP004539.D
Acq On : 13 Jan 2021 16:04
Operator : CG/JU
Sample : M1073-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

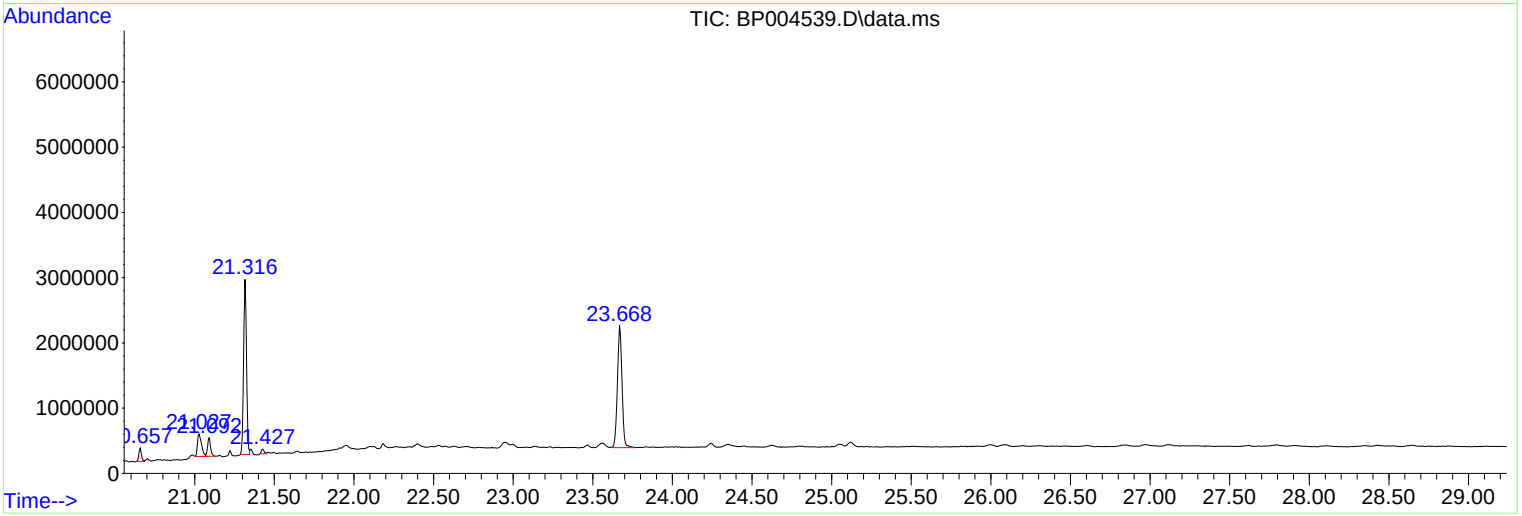
Instrument :
BNA_P
ClientSampleId :
VNJ-217

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP011221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011321\
Data File : BP004539.D
Acq On : 13 Jan 2021 16:04
Operator : CG/JU
Sample : M1073-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : VNJ-217

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP011221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

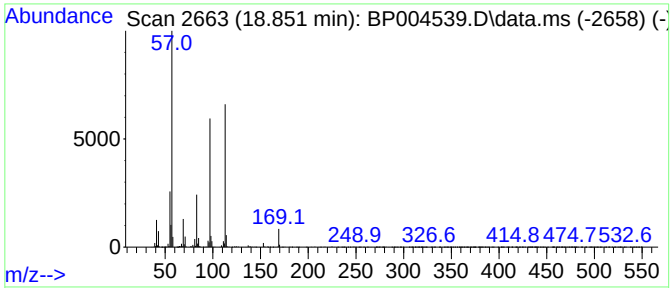
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

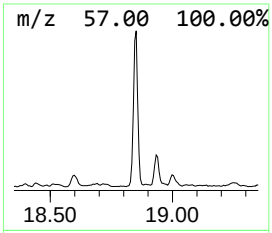
****

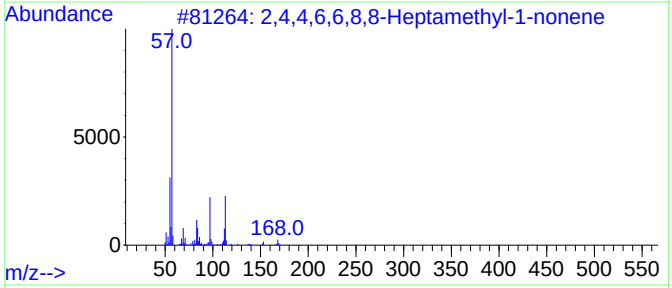
Peak Number 1 unknown18.851 Concentration Rank 2

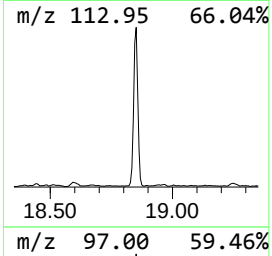
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.851	3.19 ng	405280	Phenanthrene-d10	17.222

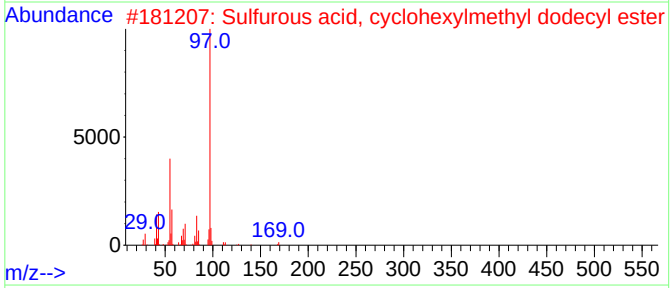
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	43
2	Sulfurous acid, cyclohexylmethyl...	346	C19H38O3S	1000309-22-0	38
3	Pyrazole, 3-nitro-	113	C3H3N3O2	026621-44-3	38
4	Octane, 2-bromo-	192	C8H17Br	000557-35-7	32
5	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	32

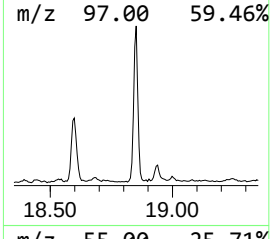


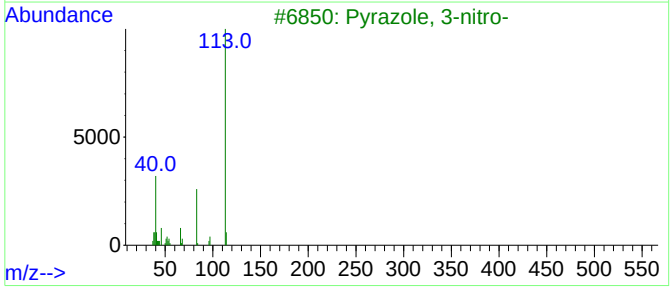


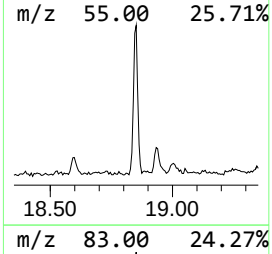


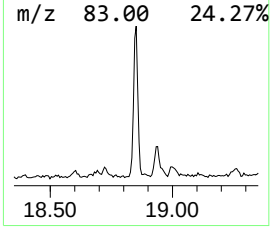












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011321\
Data File : BP004539.D
Acq On : 13 Jan 2021 16:04
Operator : CG/JU
Sample : M1073-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : VNJ-217

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP011221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

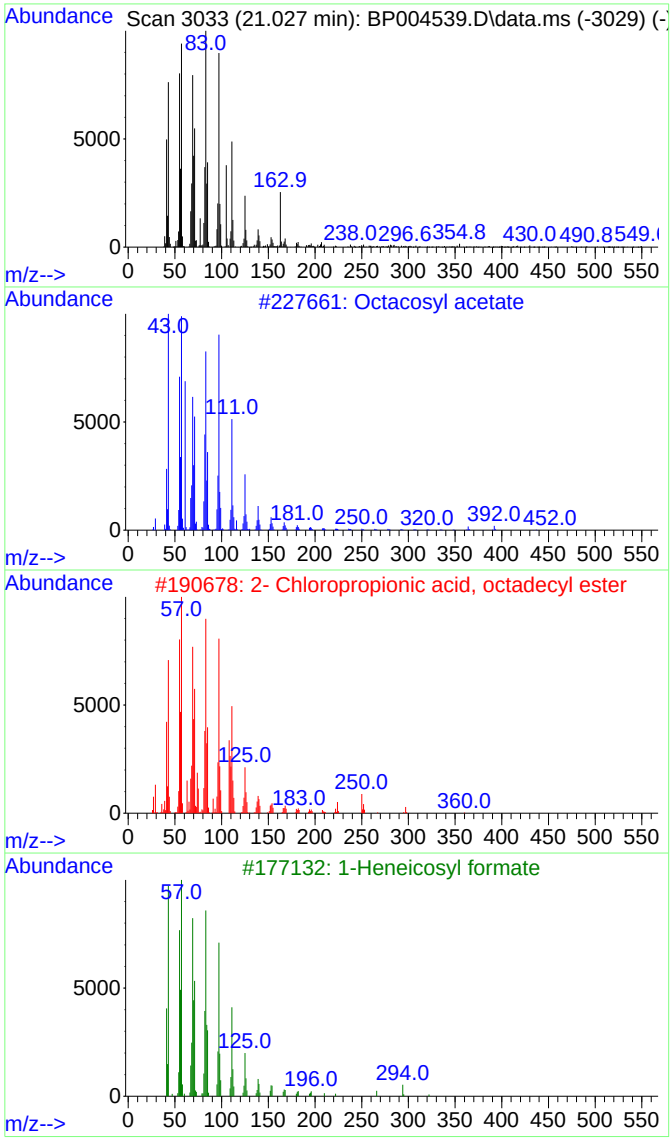
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

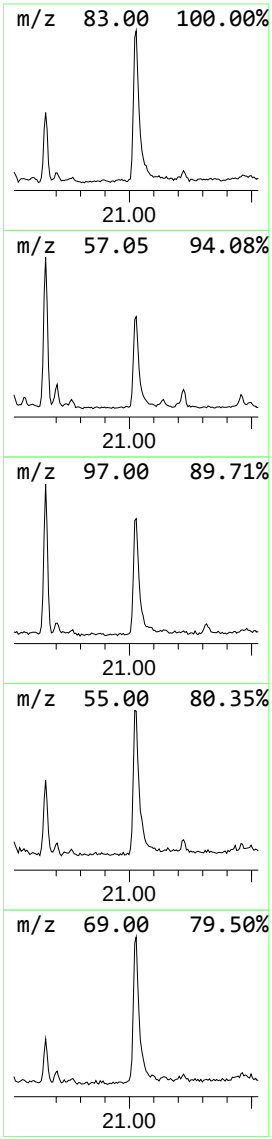
****

Peak Number 2 Octacosyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.027	3.57 ng	605815	Chrysene-d12	21.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl acetate	452	C30H60O2	018206-97-8	97
2	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
4	1-Heptacosanol	396	C27H56O	002004-39-9	93
5	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011321\
Data File : BP004539.D
Acq On : 13 Jan 2021 16:04
Operator : CG/JU
Sample : M1073-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
VNJ-217

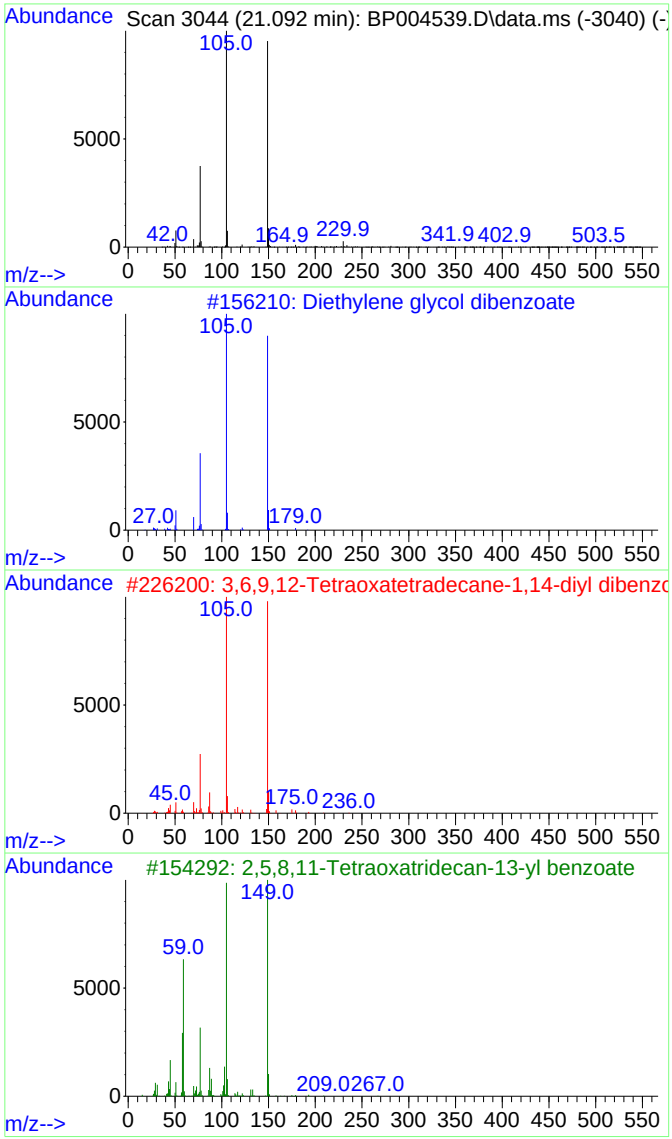
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP011221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

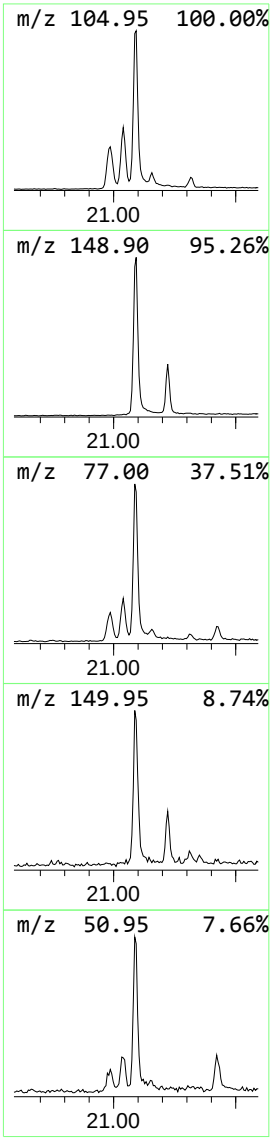
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Diethylene glycol dibenzoate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.092	2.19 ng	372010	Chrysene-d12	21.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	86
2	3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	78
3	2,5,8,11-Tetraoxatridecan-13-yl ...	312	C16H24O6	1000366-96-7	78
4	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	64
5	2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011321\
Data File : BP004539.D
Acq On : 13 Jan 2021 16:04
Operator : CG/JU
Sample : M1073-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : VNJ-217

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP011221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown18.851	18.851	3.2	ng	405280	4	17.222	2543230	20.0
Octacosyl acetate	21.027	3.6	ng	605815	5	21.316	3390220	20.0
Diethylene glyc...	21.092	2.2	ng	372010	5	21.316	3390220	20.0