LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011321\
Data File : BP004536.D
Acq On : 13 Jan 2021 14:22
Operator : CG/JU
Sample : M1058-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PB-2021-WW-000-05

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: BP004536.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.275	10	15	33	rVB	295333	435917	1.97%	0.628%
2	4.558	226	233	249	rVB	14168875	22181206	100.00%	31.977%
3	5.399	370	376	386	rBV	1228517	1840750	8.30%	2.654%
4	6.981	636	645	663	rVB2	658147	1611917	7.27%	2.324%
5	7.810	776	786	792	rBV	698018	1116925	5.04%	1.610%
6	8.969	976	983	993	rVB	1782739	2951576	13.31%	4.255%
7	10.381	1216	1223	1235	rBV	187592	349351	1.57%	0.504%
8	10.604	1254	1261	1268	rBV	823164	1419909	6.40%	2.047%
9	13.075	1673	1681	1691	rBV	4811188	7498351	33.80%	10.810%
10	13.910	1817	1823	1833	rBV	191070	293161	1.32%	0.423%
11	14.422	1904	1910	1912	rBV	446523	581832	2.62%	0.839%
12	14.463	1912	1917	1934	rVB2	1593427	3155733	14.23%	4.549%
13	15.957	2165	2171	2180	rBV	3661693	5585675	25.18%	8.053%
14	16.234	2214	2218	2221	rBV	197793	262758	1.18%	0.379%
15	17.222	2380	2386	2394	rBV	1479094	2033982	9.17%	2.932%
16	19.786	2816	2822	2834	rBV	8414790	10622409	47.89%	15.314%
17	21.022	3029	3032	3040	rBV3	437519	803470	3.62%	1.158%
18	21.092	3040	3044	3051	rVB	304614	384485	1.73%	0.554%
19	21.316	3077	3082	3087	rBV	2093292	2732691	12.32%	3.940%
20	21.739	3151	3154	3160	rVB2	152442	224740	1.01%	0.324%
21	23.668	3475	3482	3490	rBV2	1579034	3278516	14.78%	4.726%

Sum of corrected areas: 69365354

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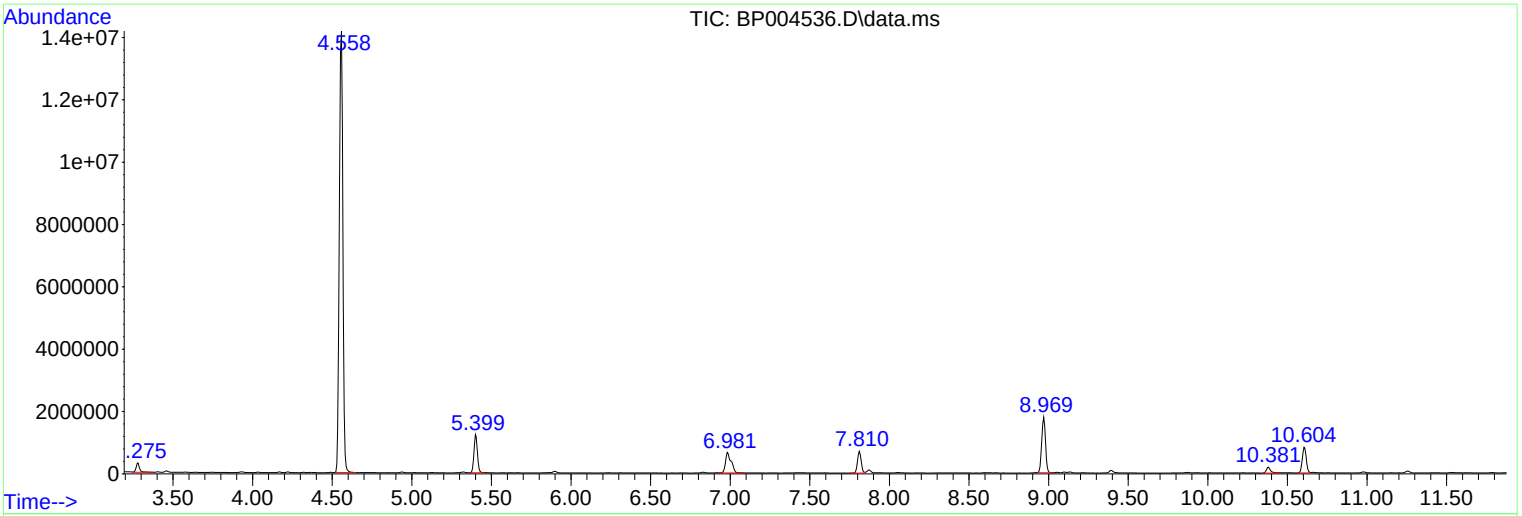
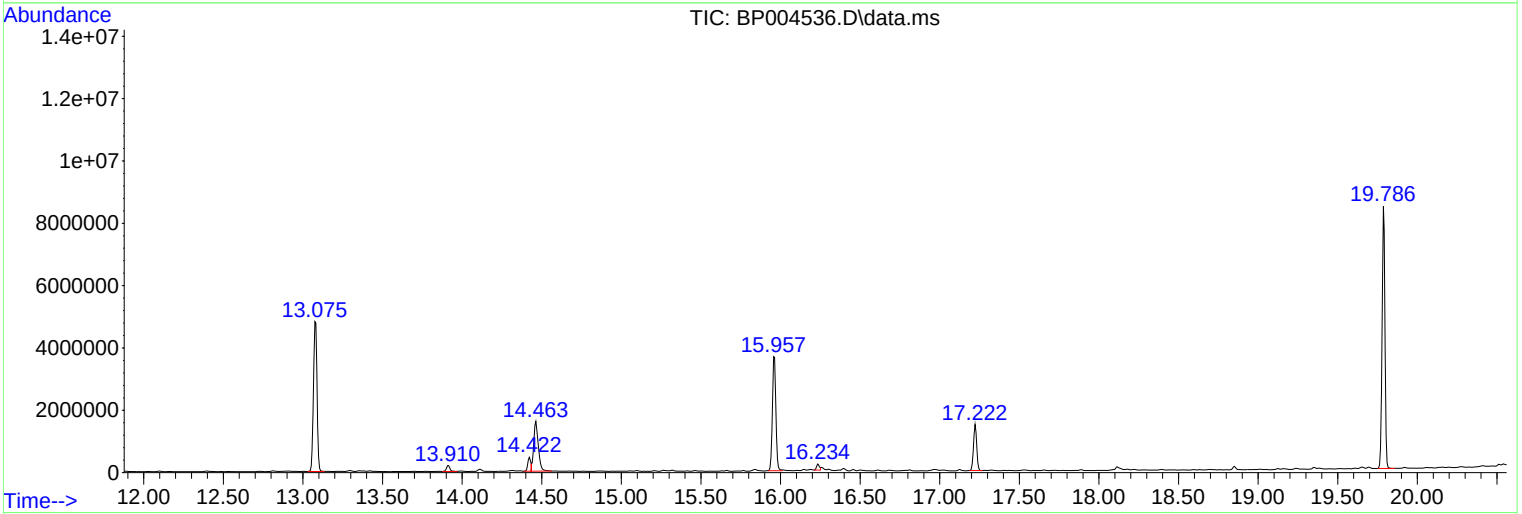
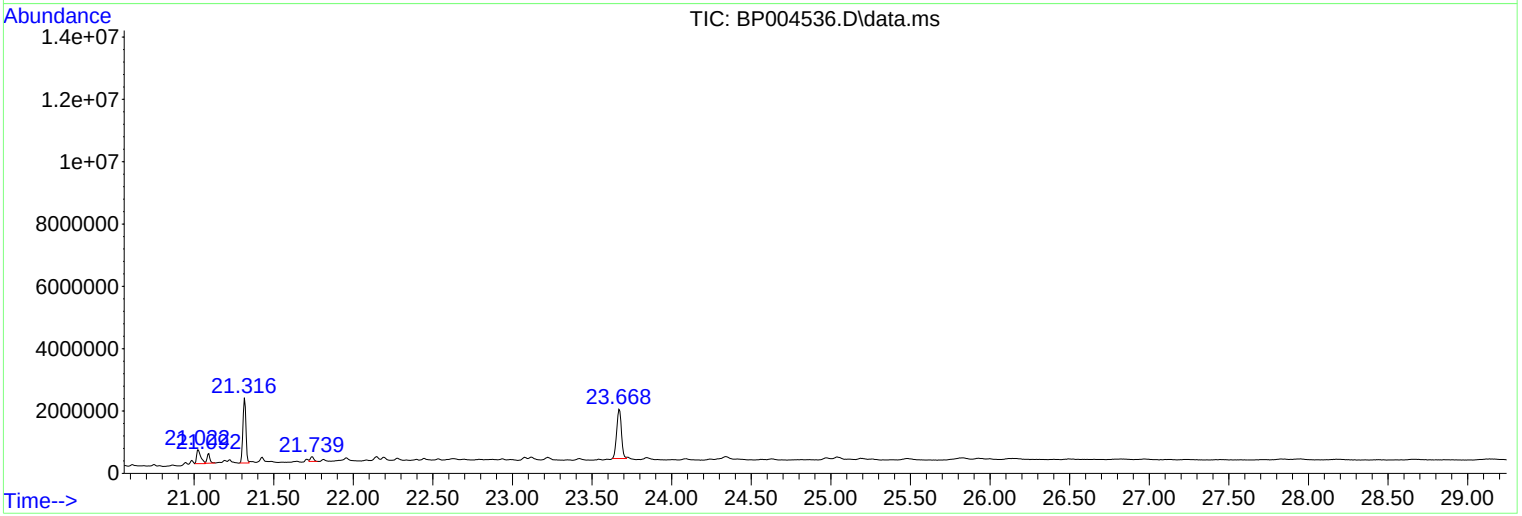
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP011221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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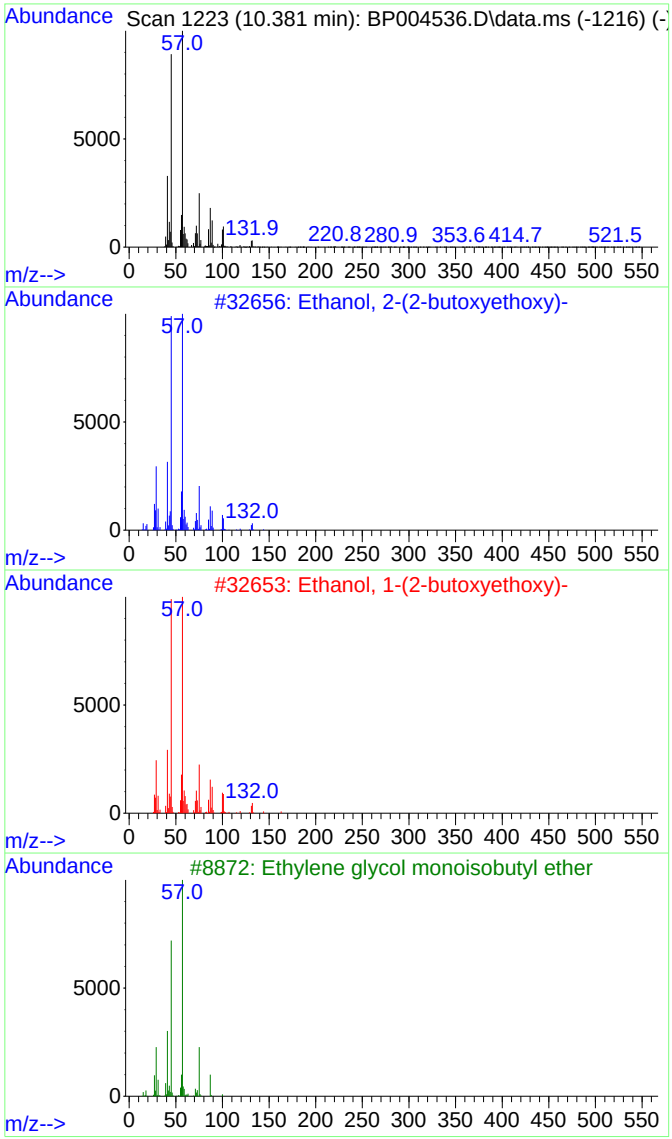
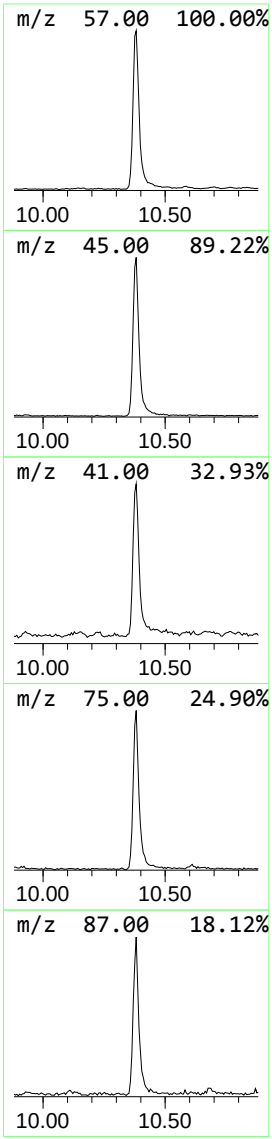
****
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.381	4.92 ng	349351	Naphthalene-d8	10.604

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	49
5	Di-sec-butyl ether	130	C8H18O	006863-58-7	47





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ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PB-2021-WW-000-05

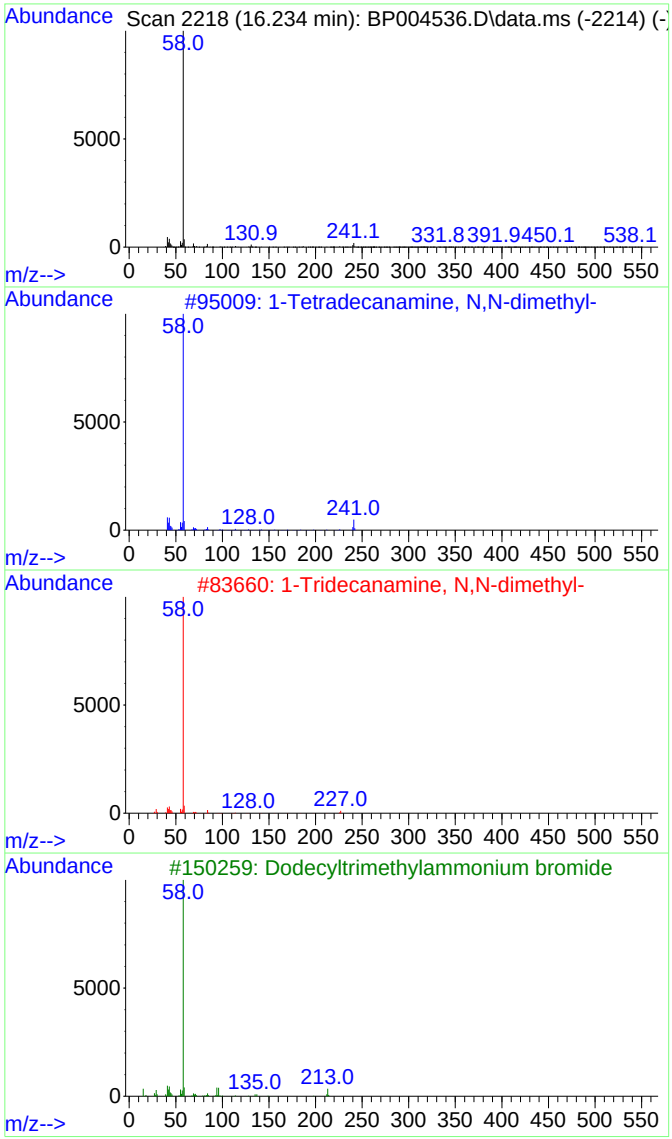
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP011221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

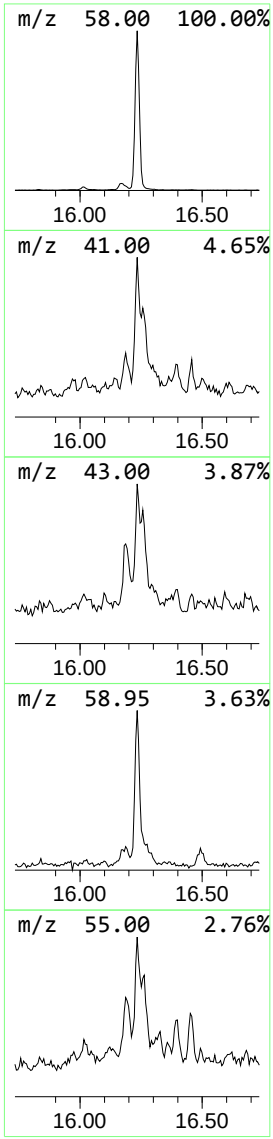
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Tetradecanamine, N,N-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.233	2.58 ng	262758	Phenanthrene-d10	17.222

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetradecanamine, N,N-dimethyl-	241	C16H35N	000112-75-4	91
2	1-Tridecanamine, N,N-dimethyl-	227	C15H33N	017373-29-4	72
3	Dodecyltrimethylammonium bromide	307	C15H34BrN	001119-94-4	72
4	1-Dodecanamine, N,N-dimethyl-	213	C14H31N	000112-18-5	72
5	Tetradonium Bromide	335	C17H38BrN	001119-97-7	72





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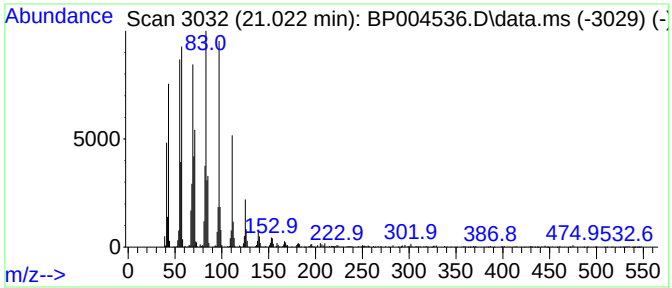
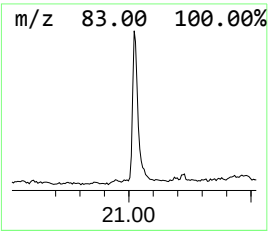
****

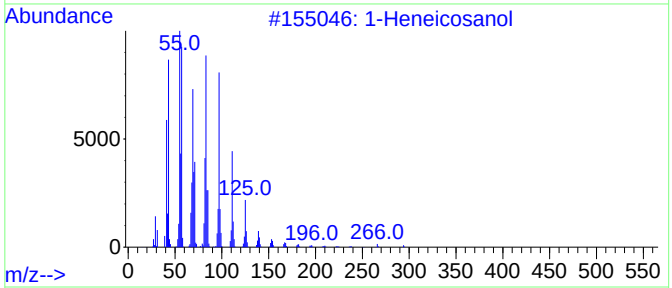
Peak Number 5 1-Heneicosanol Concentration Rank 3

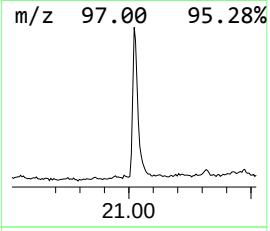
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.022	5.88 ng	803470	Chrysene-d12	21.316

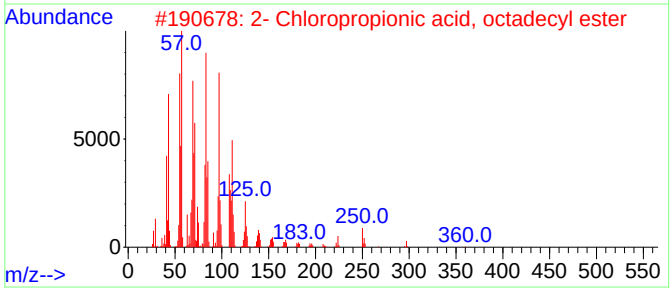
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	95
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
5	Behenic alcohol	326	C22H46O	000661-19-8	94

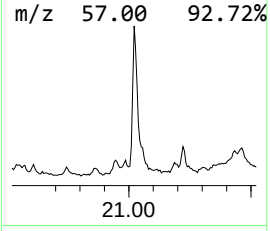


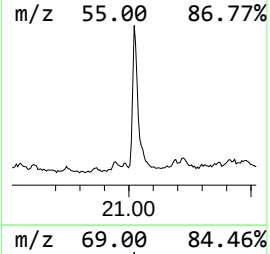


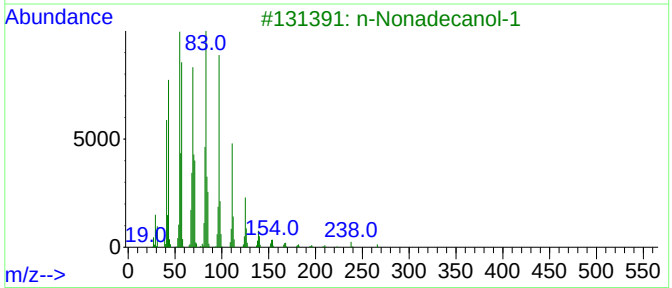


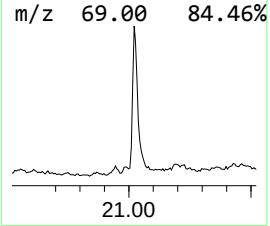












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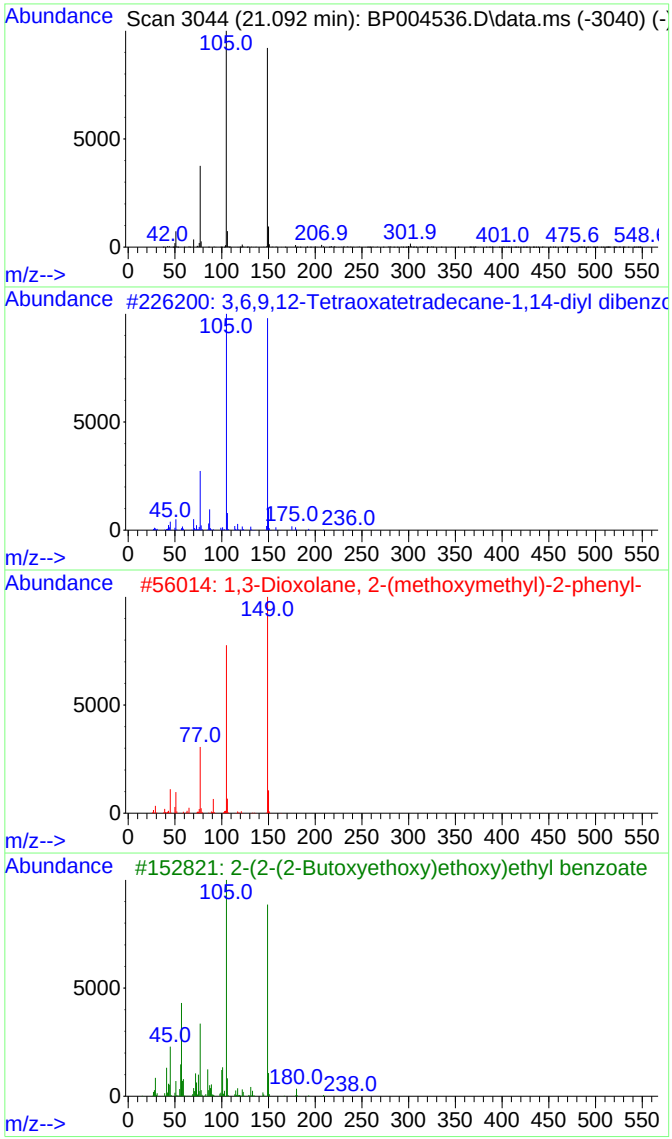
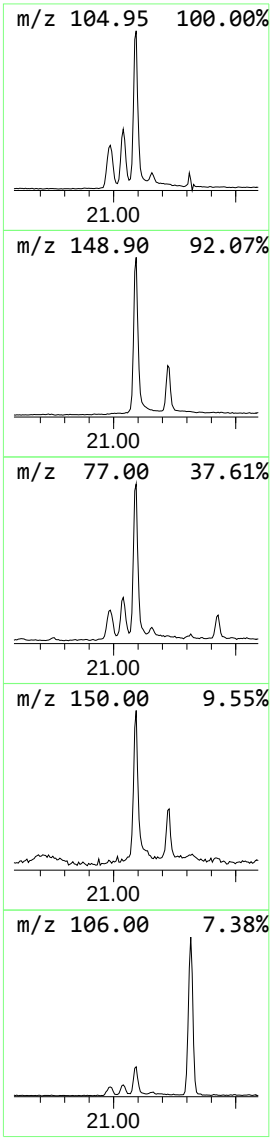
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 3,6,9,12-Tetraoxatetradecan... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.092	2.81 ng	384485	Chrysene-d12	21.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	78
2	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	72
3	2-(2-(2-Butoxyethoxy)ethoxy)ethy...	310	C17H26O5	1000366-97-2	64
4	2,5,8,11-Tetraoxatridecan-13-yl ...	312	C16H24O6	1000366-96-7	64
5	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	64





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethanol, 2-(2-b...	10.381	4.9	ng	349351	2	10.604	1419910	20.0
1-Tetradecanami...	16.233	2.6	ng	262758	4	17.222	2033980	20.0
1-Heneicosanol	21.022	5.9	ng	803470	5	21.316	2732690	20.0
3,6,9,12-Tetrao...	21.092	2.8	ng	384485	5	21.316	2732690	20.0