LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061121\
Data File : BP005882.D
Acq On : 11 Jun 2021 21:29
Operator : CG/JU
Sample : M2625-15
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 18-B12(194-198)

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-BP060821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005882.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.046	329	333	340	rVB	29374	43799	1.38%	0.358%
2	5.510	405	412	425	rBV	472309	730457	23.02%	5.970%
3	7.110	676	684	701	rBV	495320	896150	28.24%	7.325%
4	7.240	701	706	719	rVB	32261	77091	2.43%	0.630%
5	7.946	819	826	835	rBV	219985	353215	11.13%	2.887%
6	8.604	932	938	951	rBV	41119	93097	2.93%	0.761%
7	9.104	1016	1023	1036	rBV	312974	544681	17.17%	4.452%
8	10.540	1260	1267	1290	rBV2	32844	96497	3.04%	0.789%
9	10.751	1294	1303	1312	rBV	251348	444727	14.02%	3.635%
10	12.028	1512	1520	1534	rBV2	32669	74088	2.33%	0.606%
11	13.040	1687	1692	1703	rBV4	11982	34193	1.08%	0.279%
12	13.198	1712	1719	1737	rBV	1218193	1772778	55.87%	14.490%
13	13.998	1848	1855	1863	rBV	27986	50150	1.58%	0.410%
14	14.569	1945	1952	1971	rBV	369476	592057	18.66%	4.839%
15	16.063	2200	2206	2226	rBV	96200	168903	5.32%	1.381%
16	17.316	2412	2419	2435	rBV	465831	738281	23.27%	6.034%
17	19.863	2846	2852	2864	rBV	2530305	3173123	100.00%	25.936%
18	21.092	3057	3061	3069	rBV2	80606	137377	4.33%	1.123%
19	21.386	3106	3111	3118	rBV	731795	1014434	31.97%	8.291%
20	23.804	3515	3522	3532	rVB	569357	1199531	37.80%	9.804%

Sum of corrected areas: 12234629

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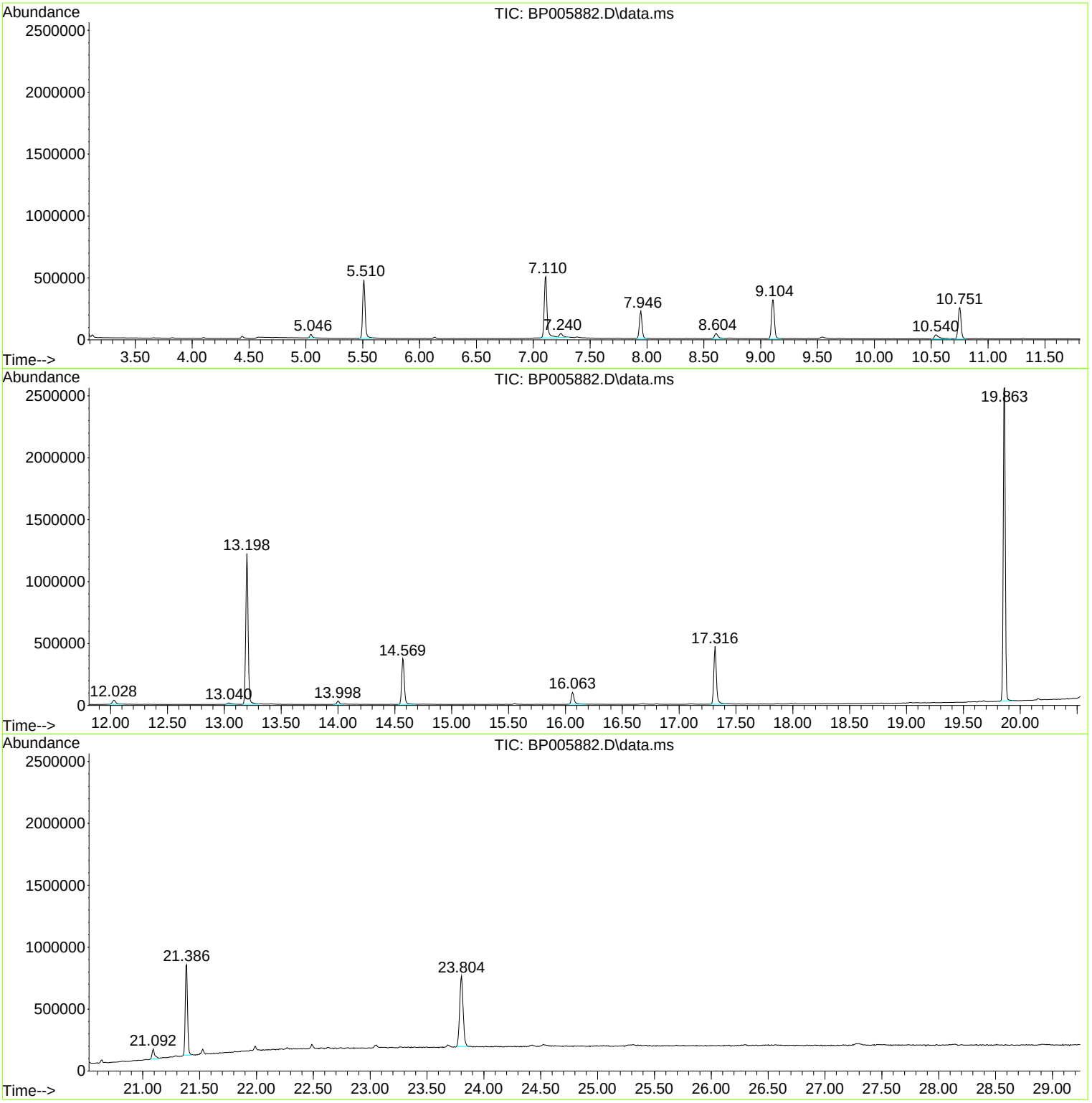
BNA_P
ClientSampleId :
18-B12(194-198)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.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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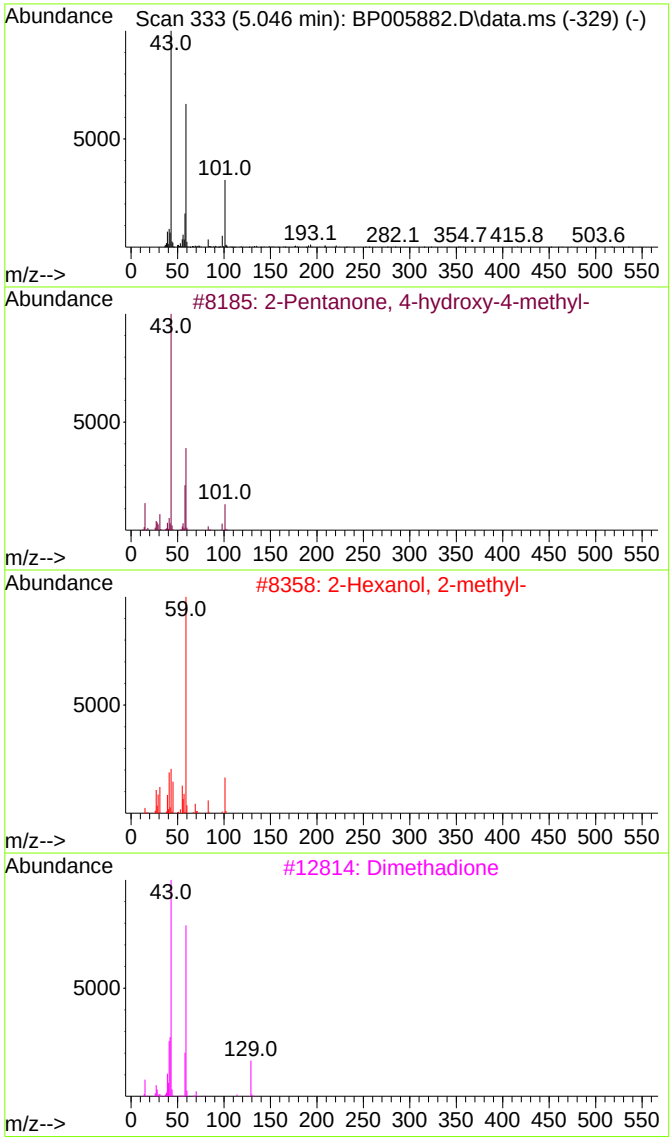
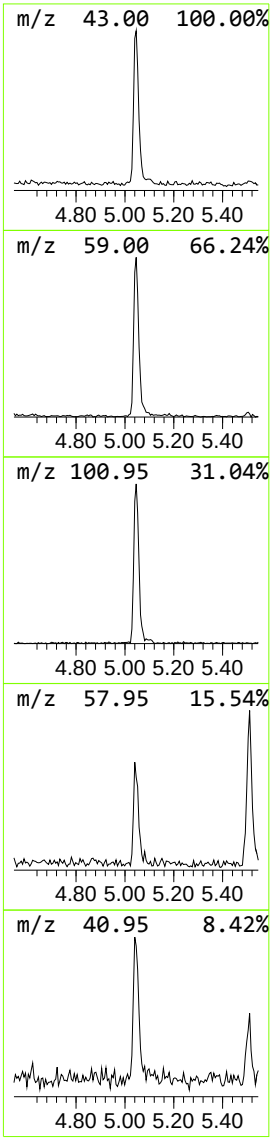
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.046	2.48 ng	43799	1,4-Dichlorobenzene-d4	7.946

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3	Dimethadione	129	C5H7NO3	000695-53-4	33
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	25
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	16





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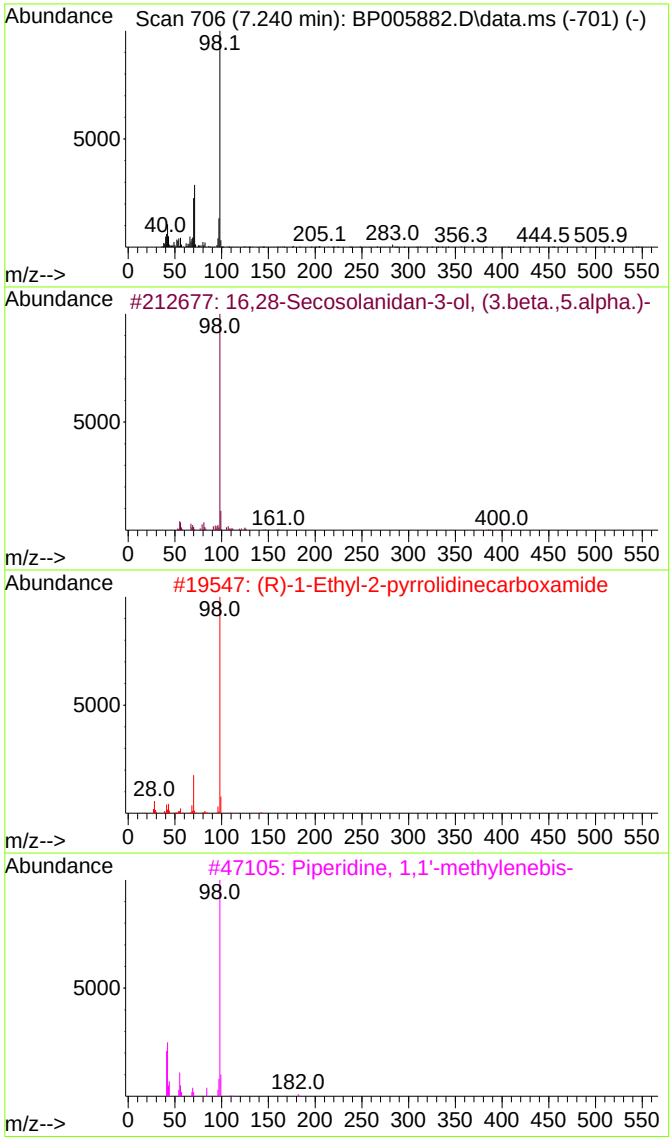
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

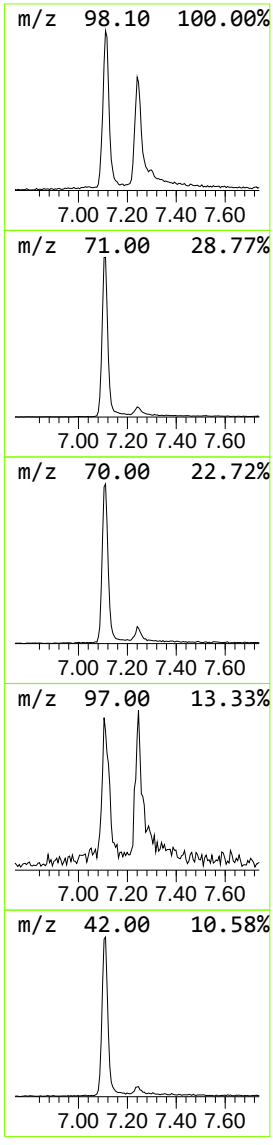
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 16,28-Secosolanidan-3-ol, (... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.240	4.37 ng	77091	1,4-Dichlorobenzene-d4	7.946

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	16,28-Secosolanidan-3-ol, (3.bet...	401	C27H47NO	030788-42-2	50
2	(R)-1-Ethyl-2-pyrrolidinecarboxa...	142	C7H14N2O	1000237-69-9	42
3	Piperidine, 1,1'-methylenebis-	182	C11H22N2	000880-09-1	40
4	2,3-2H-4-Methyl-imidazole-2-one	98	C4H6N2O	039799-77-4	40
5	Benzamide, 4-fluoro-N-[2-[1-pipe...	250	C14H19FN2O	1000128-96-4	40





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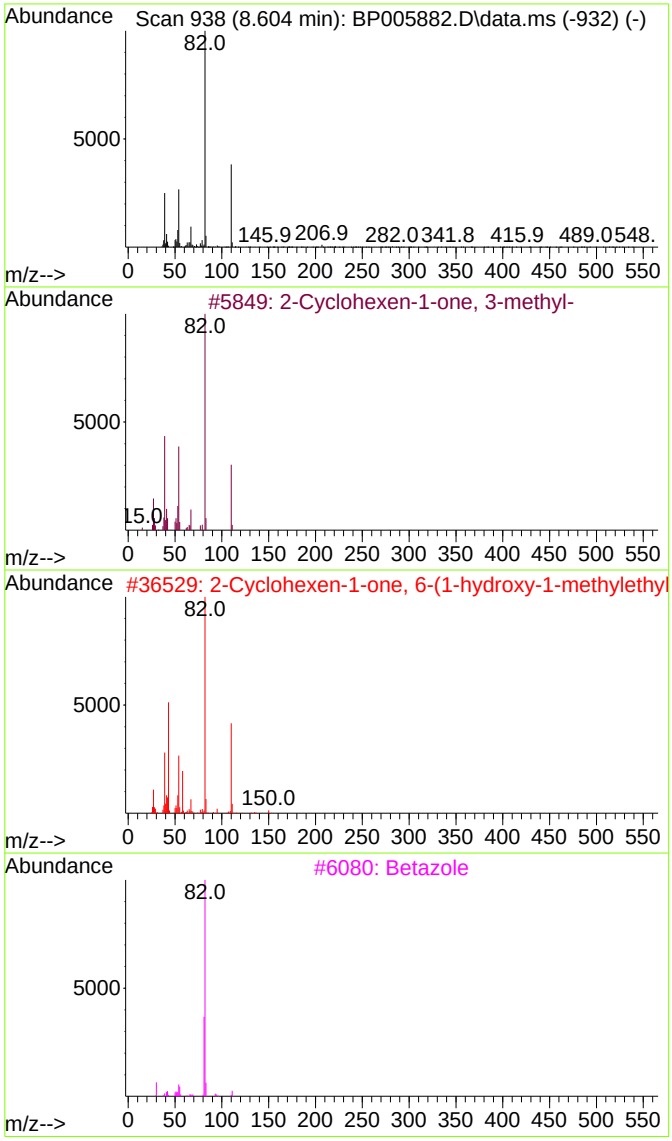
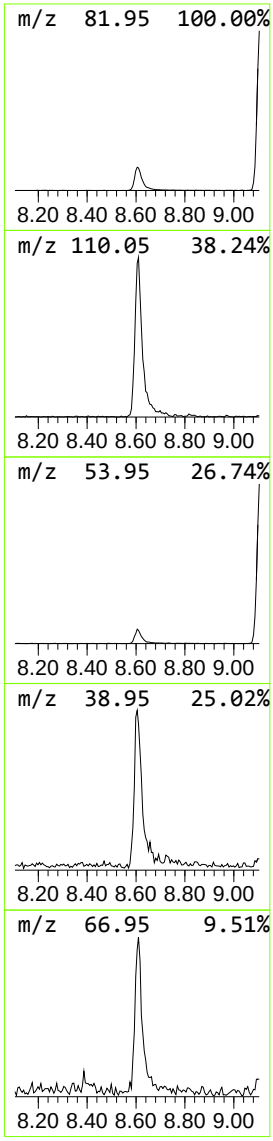
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.604	5.27 ng	93097	1,4-Dichlorobenzene-d4	7.946

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	91
2	2-Cyclohexen-1-one, 6-(1-hydroxy...	168	C10H16O2	087791-00-2	43
3	Betazole	111	C5H9N3	000105-20-4	43
4	2-Cyclohexen-1-one, 3,5-dimethyl-	124	C8H12O	001123-09-7	40
5	1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	33





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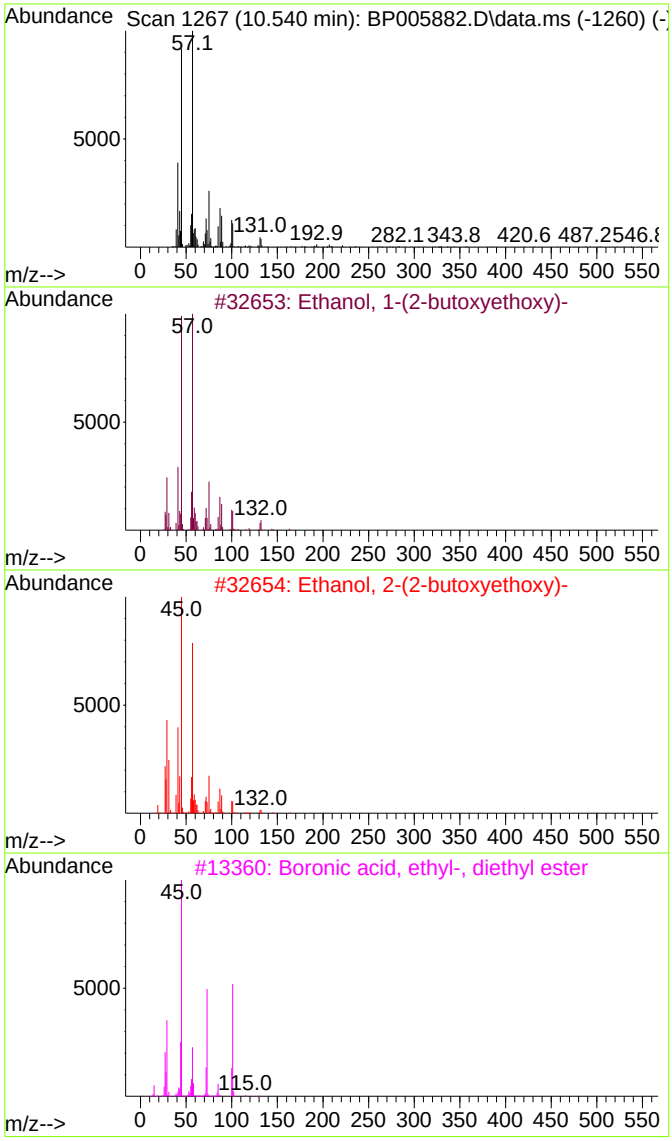
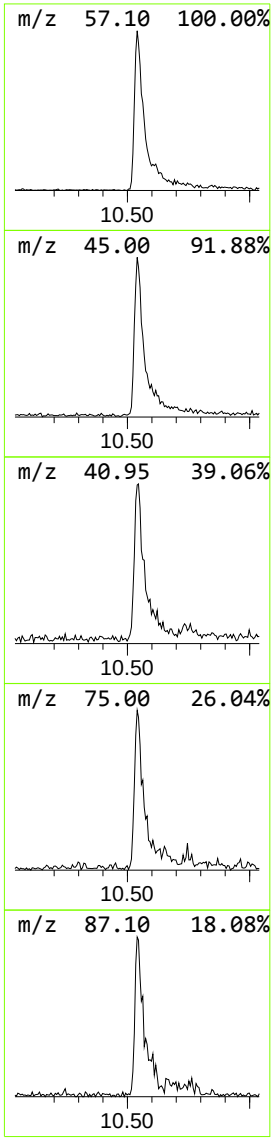
****
Peak Number 4 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.540	4.34 ng	96497	Naphthalene-d8	10.751

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
3	Boronic acid, ethyl-, diethyl ester	130	C6H15BO2	053907-92-9	47
4	5-O-Methyl-d-gluconic acid dimet...	237	C9H19NO6	013096-67-8	47
5	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	42





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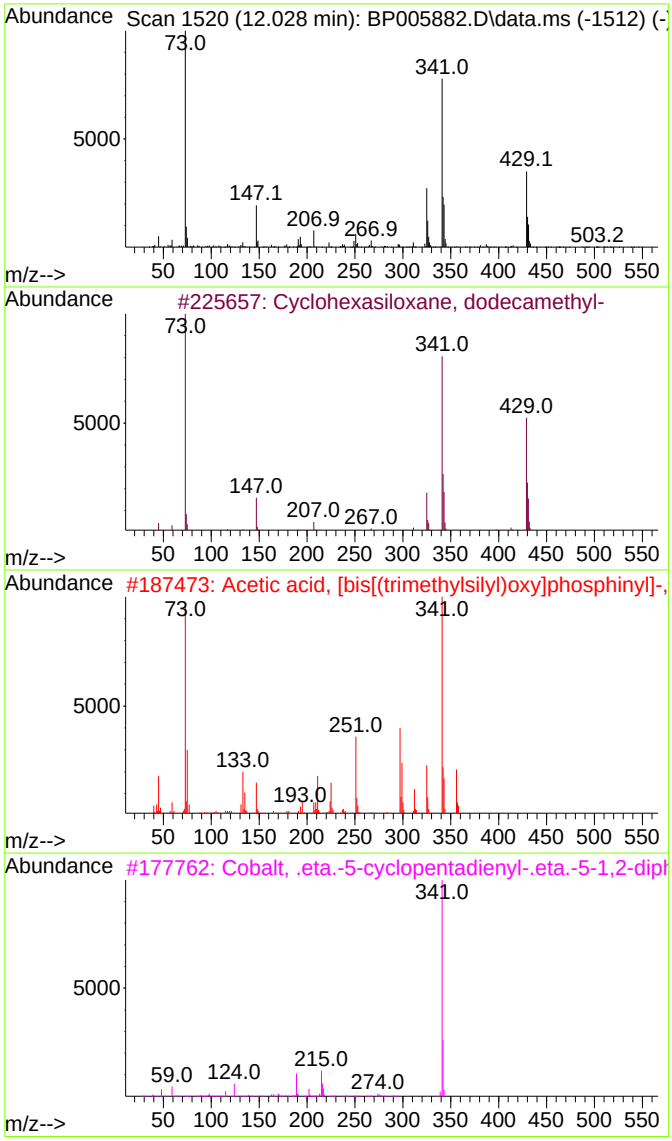
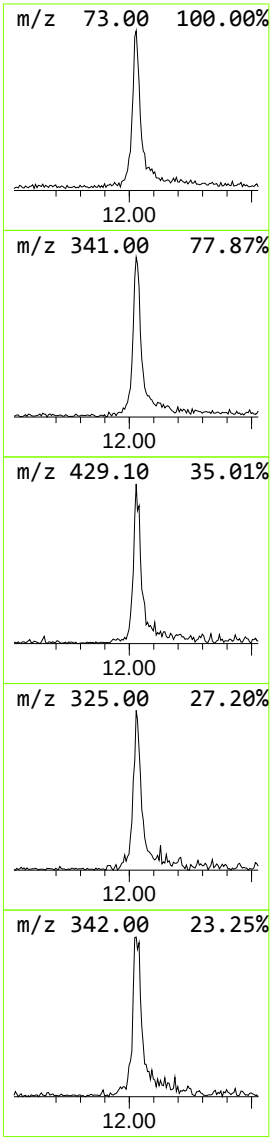
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclohexasiloxane, dodecame... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.028	3.33 ng	74088	Naphthalene-d8	10.751

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexasiloxane, dodecamethyl-	444	C12H36O6Si6	000540-97-6	90
2	Acetic acid, [bis[(trimethylsily...	356	C11H29O5PSi3	053044-27-2	42
3	Cobalt, .eta.-5-cyclopentadienyl...	341	C22H18Co	1000161-22-8	35
4	1H-Indole, 1,3-dimethyl-5,6-dime...	341	C20H23NO4	156785-76-1	35
5	Silane, dimethyl(dimethyl(dimeth...	476	C24H40O4Si3	1000347-25-6	32





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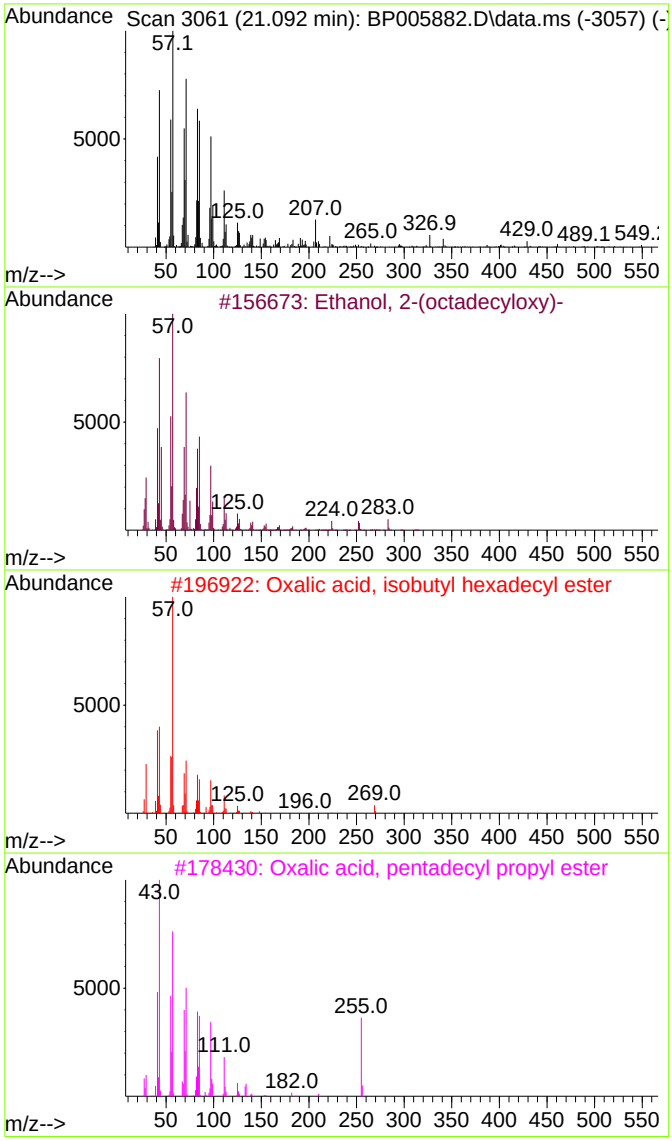
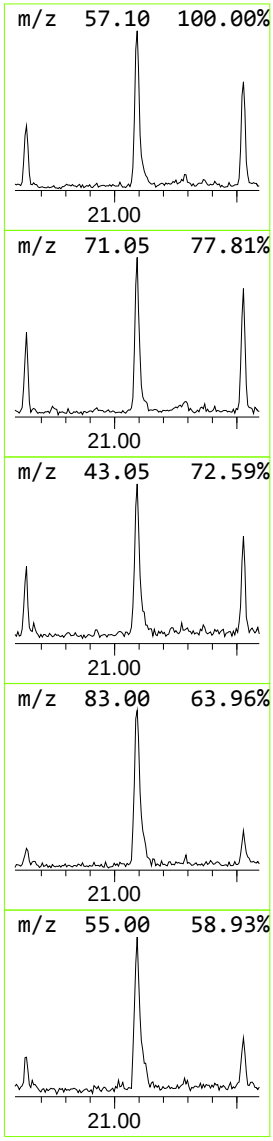
****

Peak Number 6 Ethanol, 2-(octadecyloxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.092	2.71 ng	137377	Chrysene-d12	21.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	93
2	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
3	Oxalic acid, pentadecyl propyl e...	342	C20H38O4	1000309-26-8	91
4	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	87
5	Cyclotetradecane	196	C14H28	000295-17-0	86





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.046	2.5	ng	43799	1	7.946	353215	20.0
16,28-Secosolan...	7.240	4.4	ng	77091	1	7.946	353215	20.0
2-Cyclohexen-1-...	8.604	5.3	ng	93097	1	7.946	353215	20.0
Ethanol, 1-(2-b...	10.540	4.3	ng	96497	2	10.751	444727	20.0
Cyclohexasiloxa...	12.028	3.3	ng	74088	2	10.751	444727	20.0
Ethanol, 2-(oct...	21.092	2.7	ng	137377	5	21.386	1014430	20.0