LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042321\
Data File : BP005393.D
Acq On : 23 Apr 2021 14:51
Operator : CG/JU
Sample : M2107-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-30-9.5-10.0

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-BP042121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005393.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.234	359	365	377	rBV	441734	646538	41.81%	8.461%
2	6.822	629	635	654	rBV	401606	656024	42.42%	8.585%
3	7.634	765	773	780	rBV	115462	176845	11.44%	2.314%
4	8.799	963	971	979	rBV	248889	411535	26.61%	5.385%
5	10.422	1239	1247	1257	rBV	119755	206006	13.32%	2.696%
6	12.910	1664	1670	1681	rBV	524533	785563	50.80%	10.280%
7	13.769	1809	1816	1821	rBV	13465	20958	1.36%	0.274%
8	14.181	1878	1886	1899	rBV6	8380	28980	1.87%	0.379%
9	14.304	1899	1907	1914	rVV	172925	259287	16.77%	3.393%
10	15.704	2137	2145	2154	rBV4	14352	29642	1.92%	0.388%
11	15.810	2156	2163	2180	rVV	497792	754230	48.77%	9.870%
12	17.069	2369	2377	2383	rBV	237374	336611	21.77%	4.405%
13	17.975	2526	2531	2540	rBV	144559	211804	13.70%	2.772%
14	19.098	2715	2722	2730	rBV5	16901	33728	2.18%	0.441%
15	19.216	2738	2742	2755	rBV2	66970	96417	6.23%	1.262%
16	19.651	2810	2816	2826	rBV	1381620	1546438	100.00%	20.237%
17	20.857	3016	3021	3023	rBV	28512	44124	2.85%	0.577%
18	20.892	3023	3027	3034	rVV2	98021	182394	11.79%	2.387%
19	20.957	3035	3038	3046	rVB	75400	100705	6.51%	1.318%
20	21.086	3058	3060	3064	rBV2	18588	20737	1.34%	0.271%
21	21.174	3070	3075	3080	rBV	388402	508737	32.90%	6.657%
22	22.345	3271	3274	3279	rVB	44831	57813	3.74%	0.757%
23	23.433	3453	3459	3470	rVB2	269352	526630	34.05%	6.891%

Sum of corrected areas: 7641746

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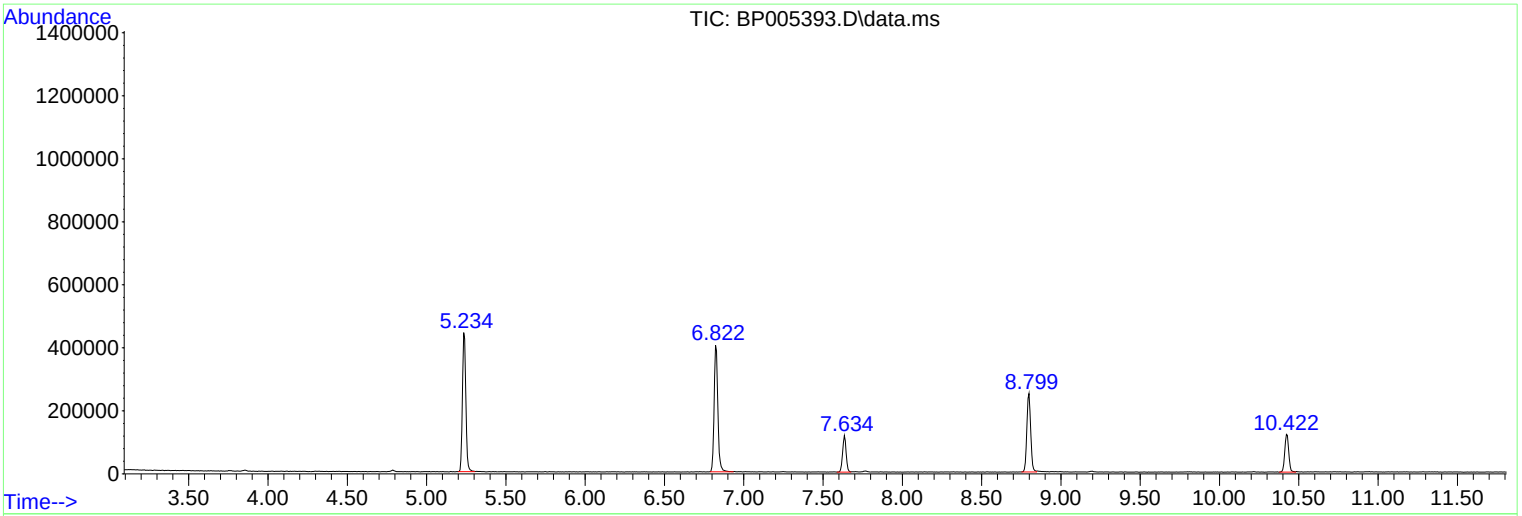
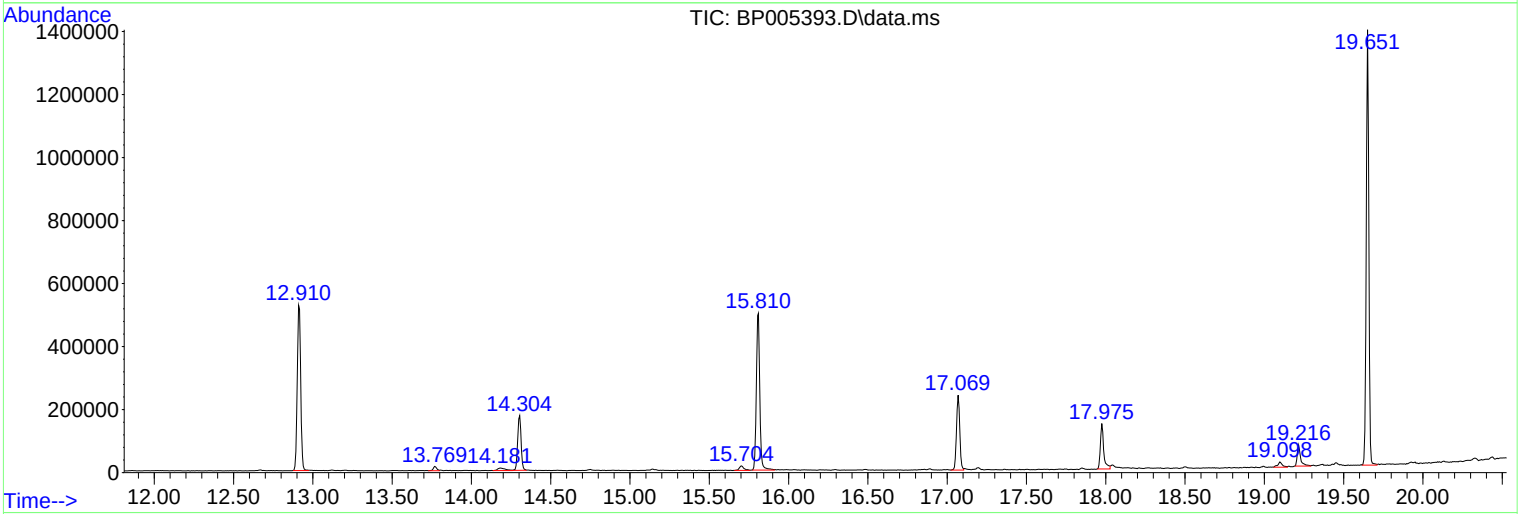
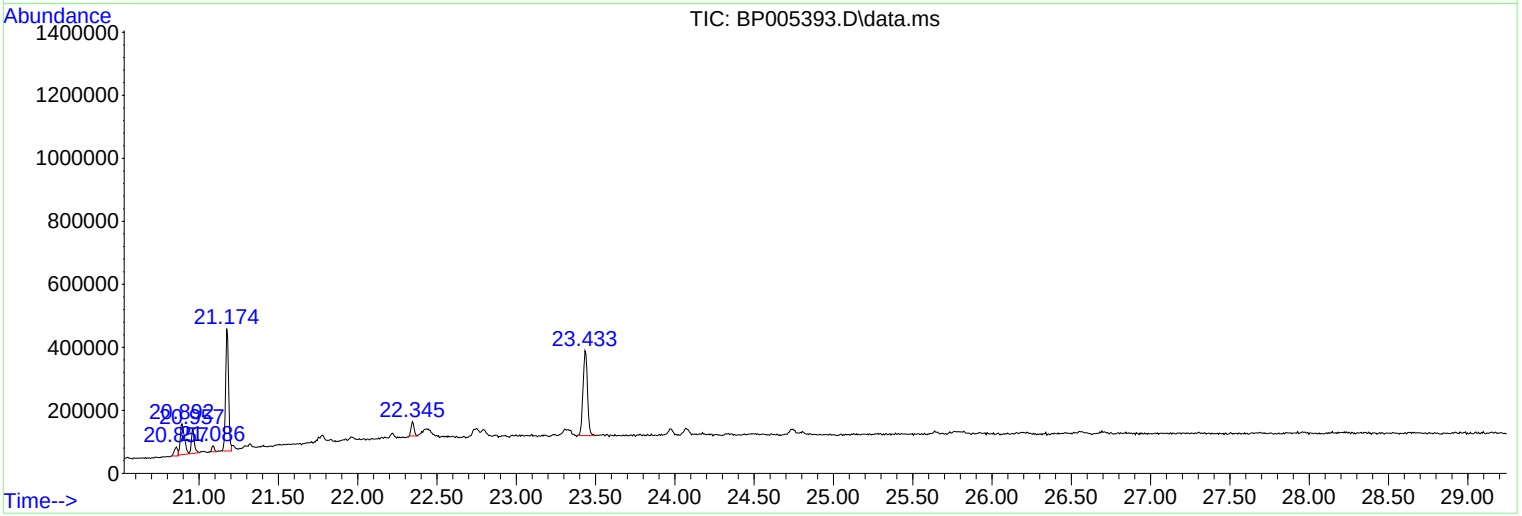
Instrument :
BNA_P
ClientSampleId :
SB-30-9.5-10.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.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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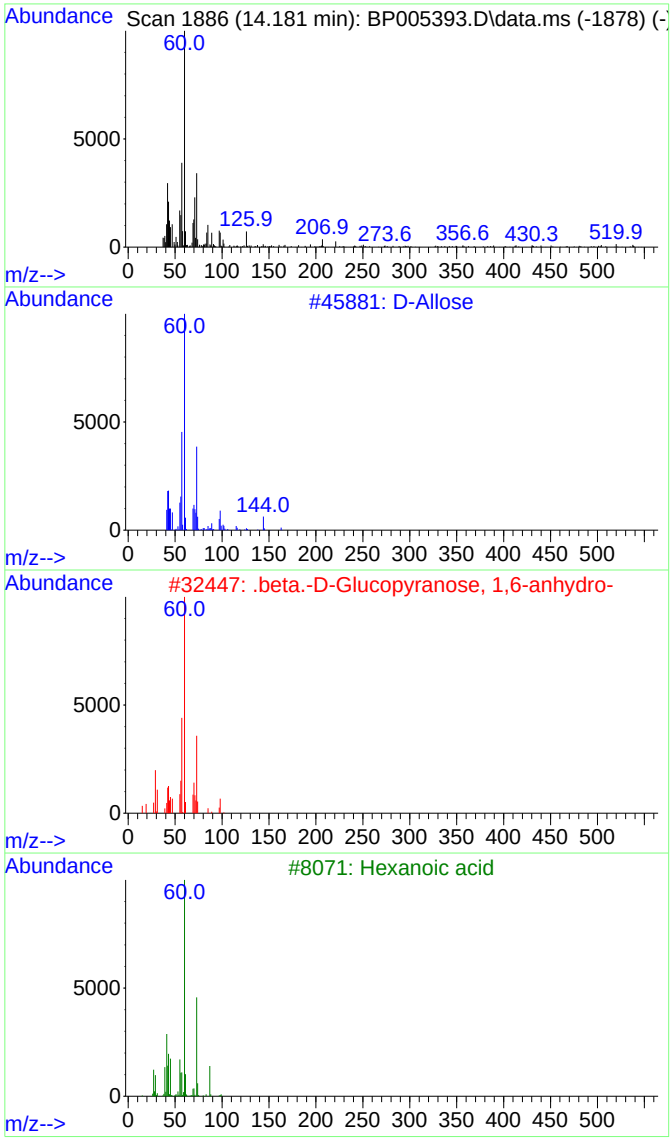
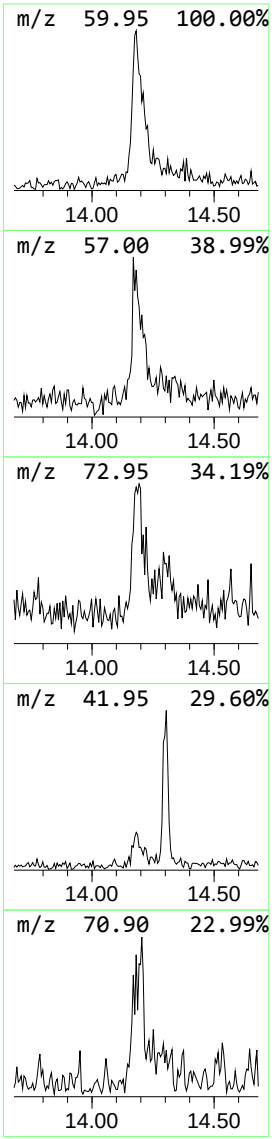
Peak Number 1 D-Allose Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.181	2.24 ng	28980	Acenaphthene-d10	14.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Allose	180	C6H12O6	002595-97-3	72
2	.beta.-D-Glucopyranose, 1,6-anhy...	162	C6H10O5	000498-07-7	64
3	Hexanoic acid	116	C6H12O2	000142-62-1	59
4	.alpha.-D-Galactopyranoside, methyl	194	C7H14O6	003396-99-4	45
5	Pentanoic acid	102	C5H10O2	000109-52-4	45





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Operator : CG/JU
Sample : M2107-06
Misc :
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Instrument : BNA_P
ClientSampleId : SB-30-9.5-10.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
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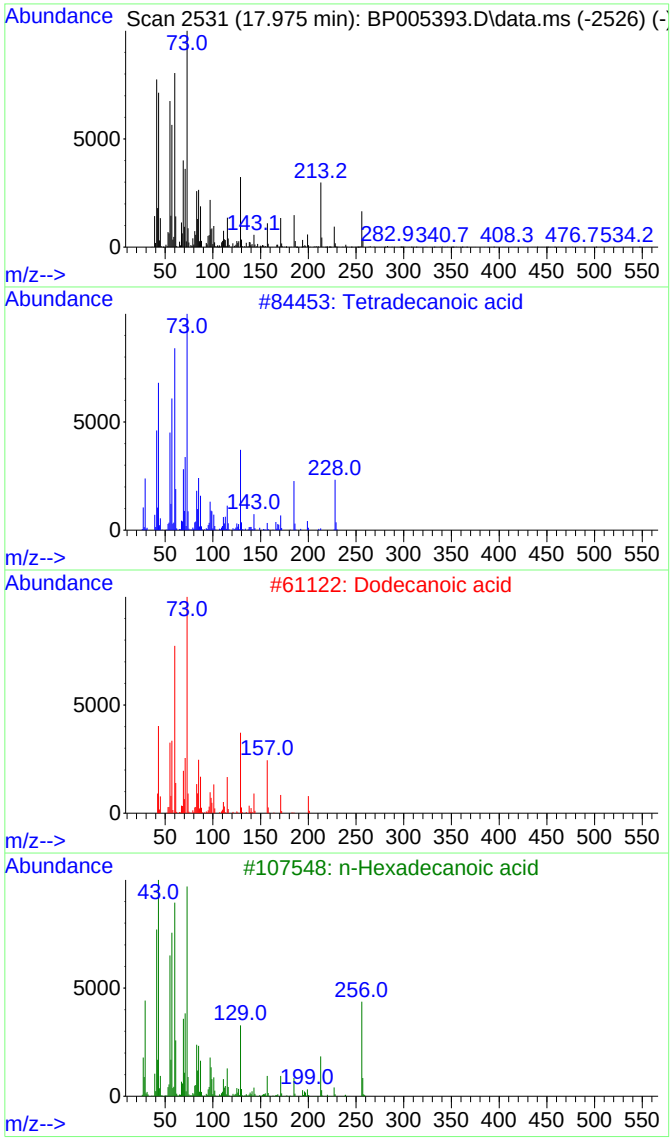
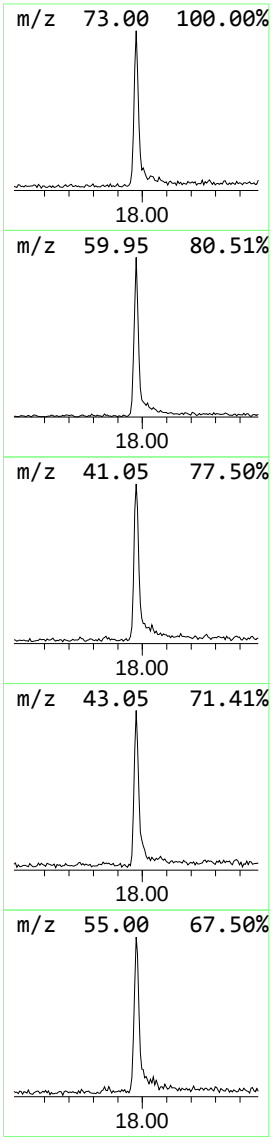
Peak Number 2 Tetradecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.975	12.58 ng	211804	Phenanthrene-d10	17.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
2	Dodecanoic acid	200	C12H24O2	000143-07-7	91
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
4	Tridecanoic acid	214	C13H26O2	000638-53-9	91
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	62





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Data File : BP005393.D
Acq On : 23 Apr 2021 14:51
Operator : CG/JU
Sample : M2107-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-30-9.5-10.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
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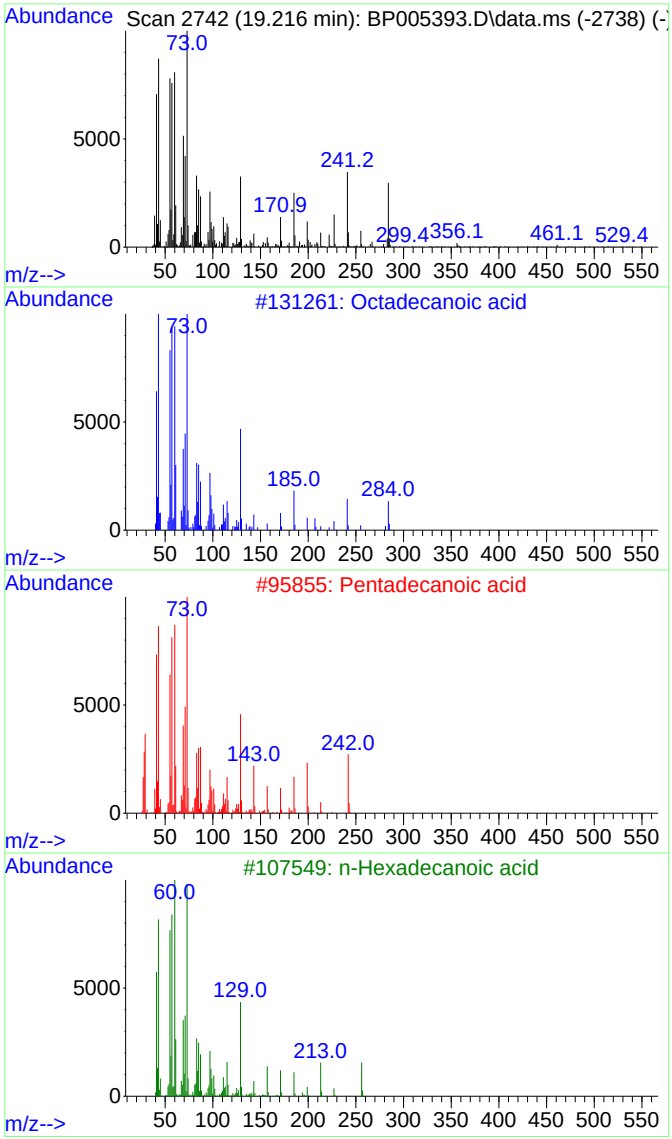
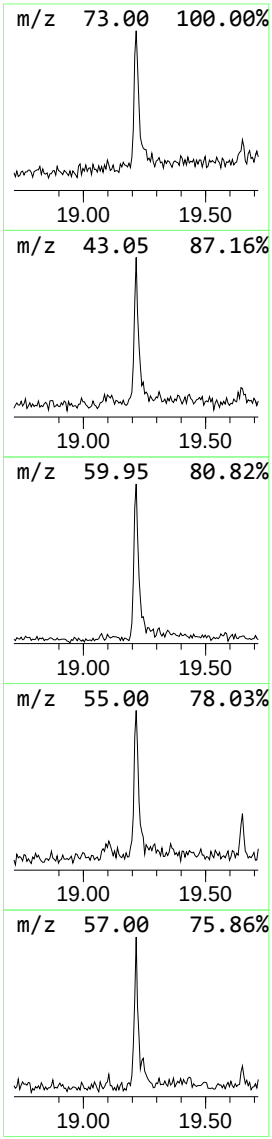
Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.216	3.79 ng	96417	Chrysene-d12	21.174

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





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Data File : BP005393.D
Acq On : 23 Apr 2021 14:51
Operator : CG/JU
Sample : M2107-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-30-9.5-10.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
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TIC Library : C:\DATABASE\NIST11.L
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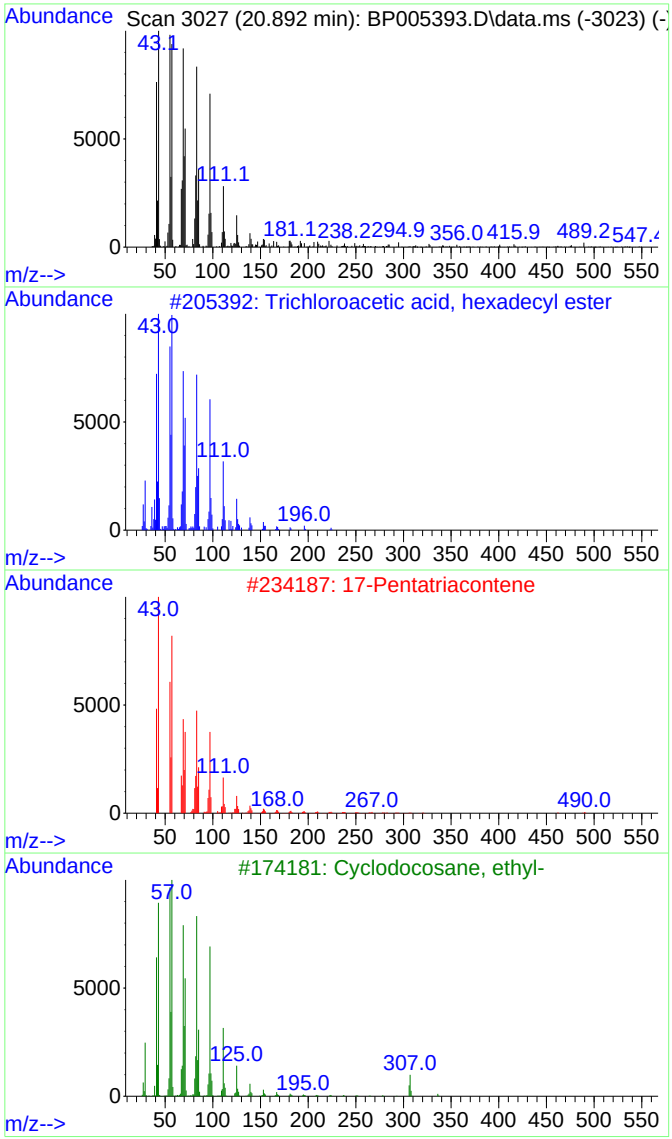
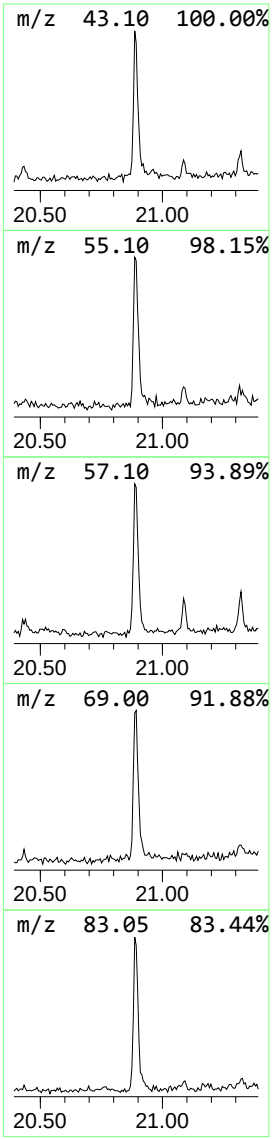
Peak Number 5 Trichloroacetic acid, hexad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.892	7.17 ng	182394	Chrysene-d12	21.174

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	17-Pentatriacontene	491	C35H70	006971-40-0	91
3	Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	90
4	Cyclotetracosane	336	C24H48	000297-03-0	89
5	8-Heptadecene	238	C17H34	002579-04-6	89





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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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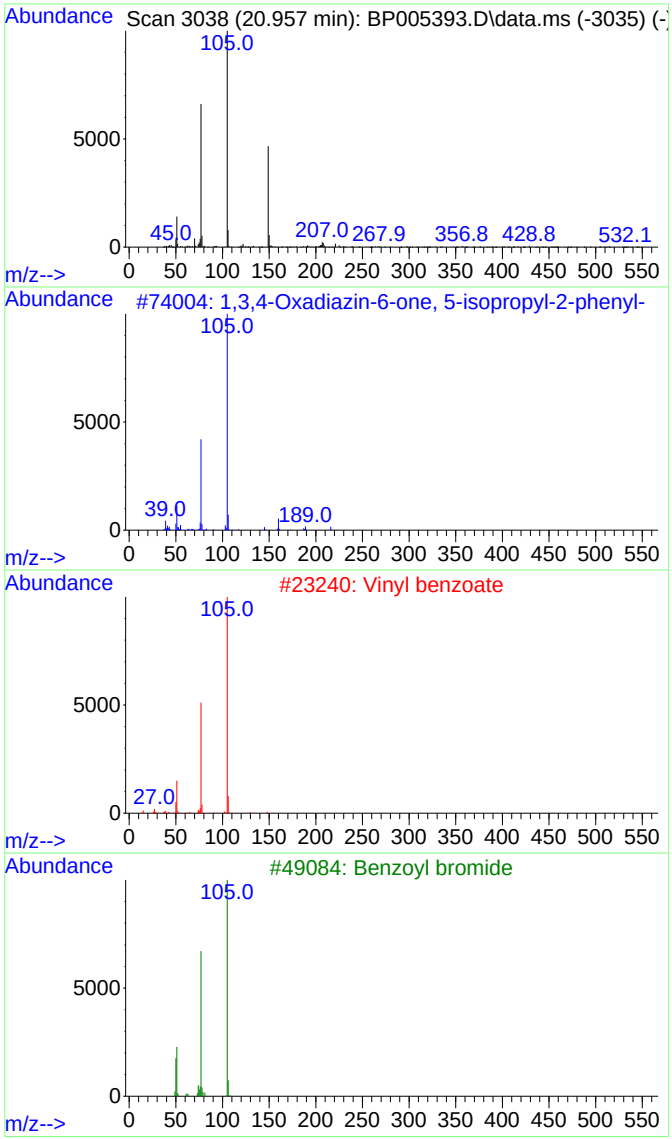
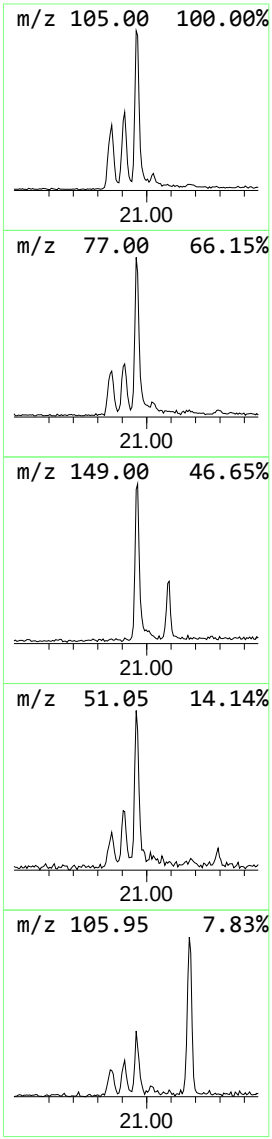
Peak Number 6 unknown20.95 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.957	3.96 ng	100705	Chrysene-d12	21.174

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,4-Oxadiazin-6-one, 5-isoprop...	216	C12H12N2O2	173973-78-9	47
2	Vinyl benzoate	148	C9H8O2	000769-78-8	47
3	Benzoyl bromide	184	C7H5BrO	000618-32-6	47
4	Benzamide, N-(5-benzylidenamino-...	368	C20H14Cl2N2O	1000263-39-7	47
5	2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	47





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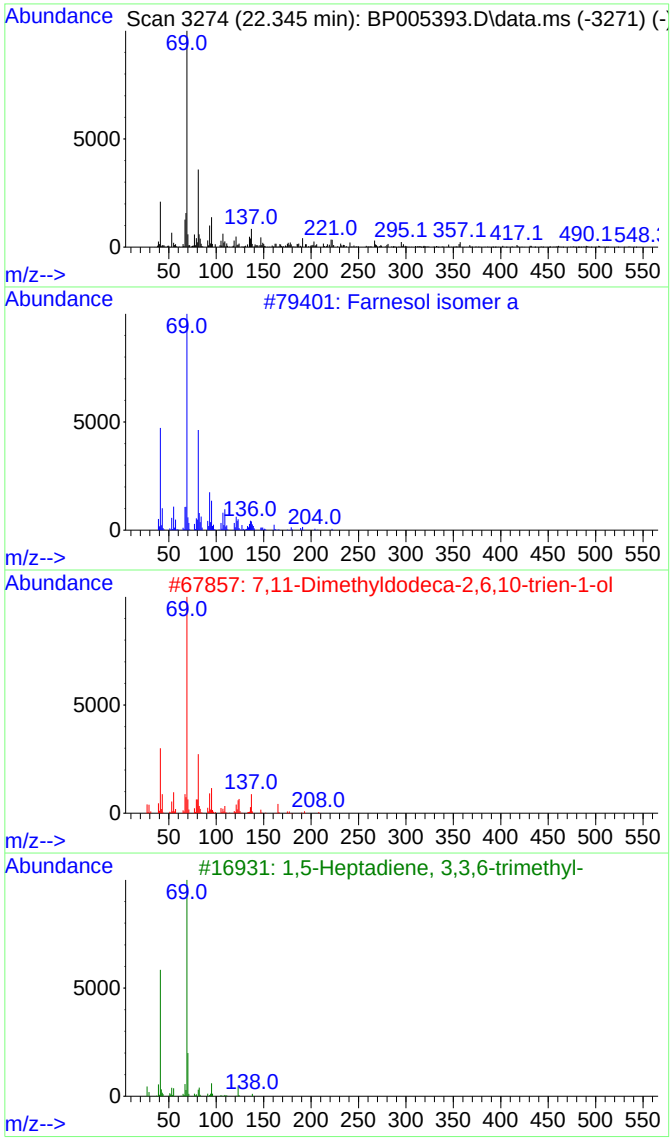
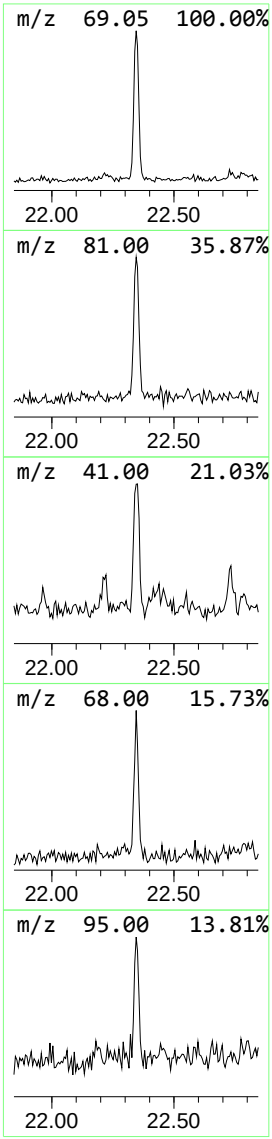
Peak Number 7 Farnesol isomer a Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.345	2.20 ng	57813	Perylene-d12	23.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Farnesol isomer a	222	C15H26O	1000108-92-4	72
2	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
3	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	64
4	Geranyl bromide	216	C10H17Br	006138-90-5	59
5	1,6-Octadien-3-ol, 3,7-dimethyl-...	182	C11H18O2	000115-99-1	59





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
D-Allose	14.181	2.2	ng	28980	3	14.304	259287	20.0
Tetradecanoic acid	17.975	12.6	ng	211804	4	17.069	336611	20.0
Octadecanoic acid	19.216	3.8	ng	96417	5	21.174	508737	20.0
Trichloroacetic...	20.892	7.2	ng	182394	5	21.174	508737	20.0
unknown20.95	20.957	4.0	ng	100705	5	21.174	508737	20.0
Farnesol isomer a	22.345	2.2	ng	57813	6	23.433	526630	20.0