LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020922\
Data File : BP009074.D
Acq On : 09 Feb 2022 13:02
Operator : CG/JU
Sample : N1421-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-1

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-BP020722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP009074.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.928	323	330	339	rBV	150737	228690	2.00%	0.378%
2	5.399	403	410	423	rBV	2542861	4008360	35.08%	6.620%
3	6.993	674	681	695	rBV	2485612	4262255	37.30%	7.039%
4	7.805	810	819	827	rBV	669485	1072494	9.39%	1.771%
5	8.969	1009	1017	1039	rVB	1608710	2760882	24.16%	4.560%
6	10.604	1287	1295	1302	rBV	898605	1542411	13.50%	2.547%
7	13.069	1707	1714	1725	rBV	4532978	7090420	62.05%	11.710%
8	14.451	1942	1949	1965	rVB	1567654	2484604	21.74%	4.103%
9	15.269	2081	2088	2093	rBV2	107704	232849	2.04%	0.385%
10	15.734	2160	2167	2176	rBV2	83665	245186	2.15%	0.405%
11	15.945	2197	2203	2216	rVB	4379289	6494133	56.84%	10.725%
12	16.610	2312	2316	2325	rVB2	118523	216668	1.90%	0.358%
13	17.204	2411	2417	2425	rBV	2163516	3138447	27.47%	5.183%
14	17.881	2528	2532	2537	rVB2	92602	126898	1.11%	0.210%
15	18.104	2565	2570	2577	rBV	663198	1000691	8.76%	1.653%
16	18.375	2612	2616	2620	rBV	214017	325738	2.85%	0.538%
17	18.416	2620	2623	2634	rVB	282007	489017	4.28%	0.808%
18	19.339	2776	2780	2792	rBV	507831	734765	6.43%	1.213%
19	19.769	2848	2853	2859	rBV	8835026	11426234	100.00%	18.870%
20	20.516	2975	2980	2990	rVB2	372836	834806	7.31%	1.379%
21	20.651	2995	3003	3015	rVV	577902	1576337	13.80%	2.603%
22	21.010	3060	3064	3072	rBV2	500027	753198	6.59%	1.244%
23	21.304	3109	3114	3119	rBV	2809064	3637391	31.83%	6.007%
24	21.369	3122	3125	3132	rVB5	185012	401071	3.51%	0.662%
25	23.498	3482	3487	3499	rVB4	493066	1485599	13.00%	2.453%
26	23.704	3515	3522	3531	rVB2	1973709	3981653	34.85%	6.576%

Sum of corrected areas: 60550797

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ClientSampleId :
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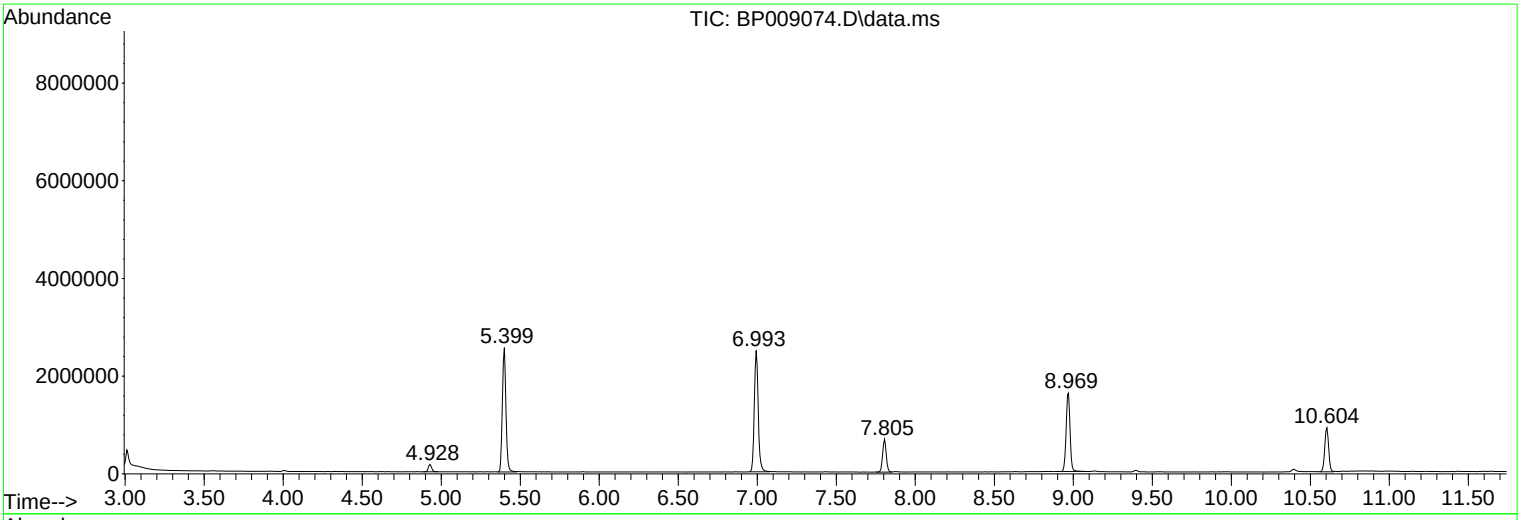
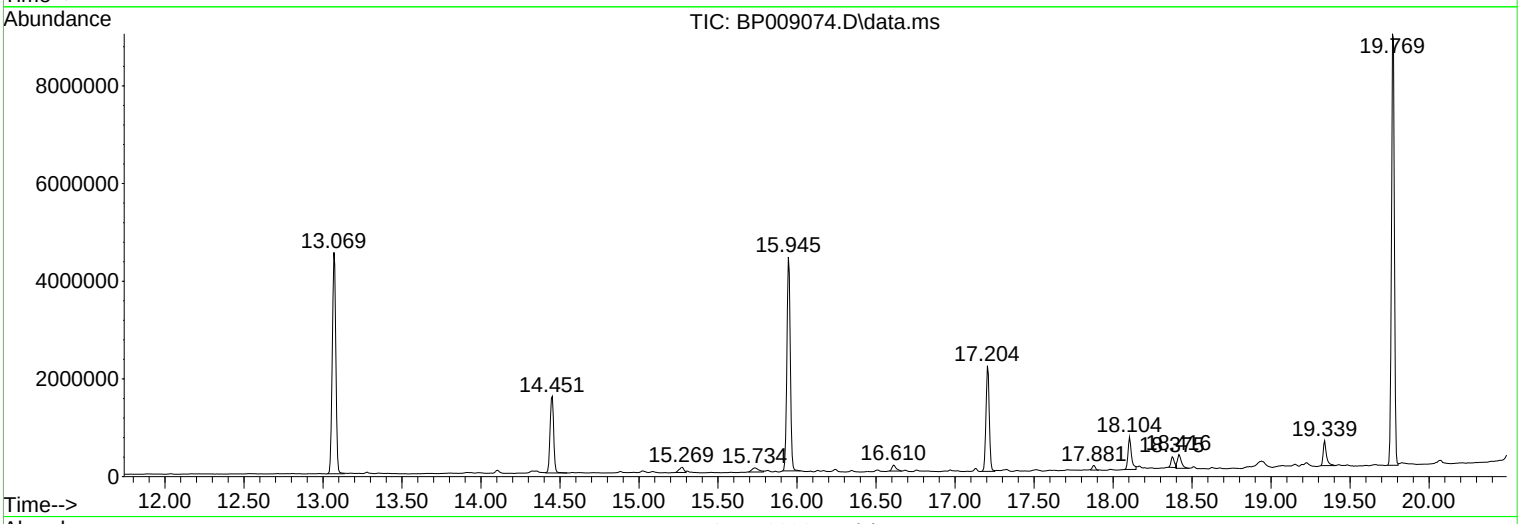
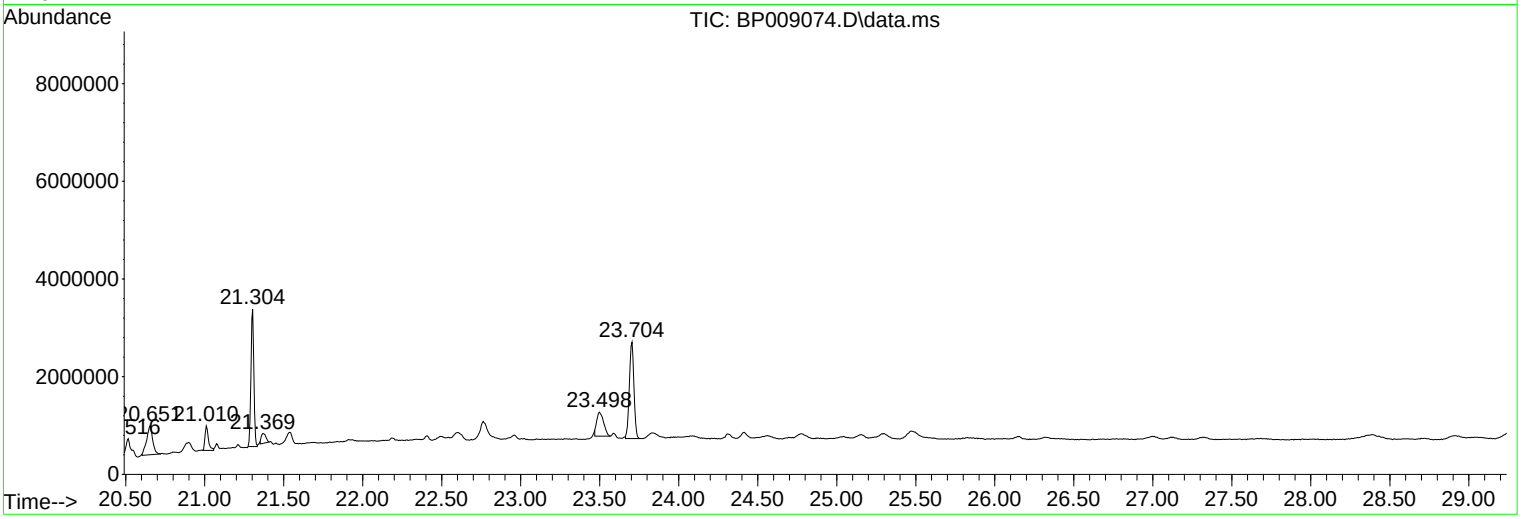
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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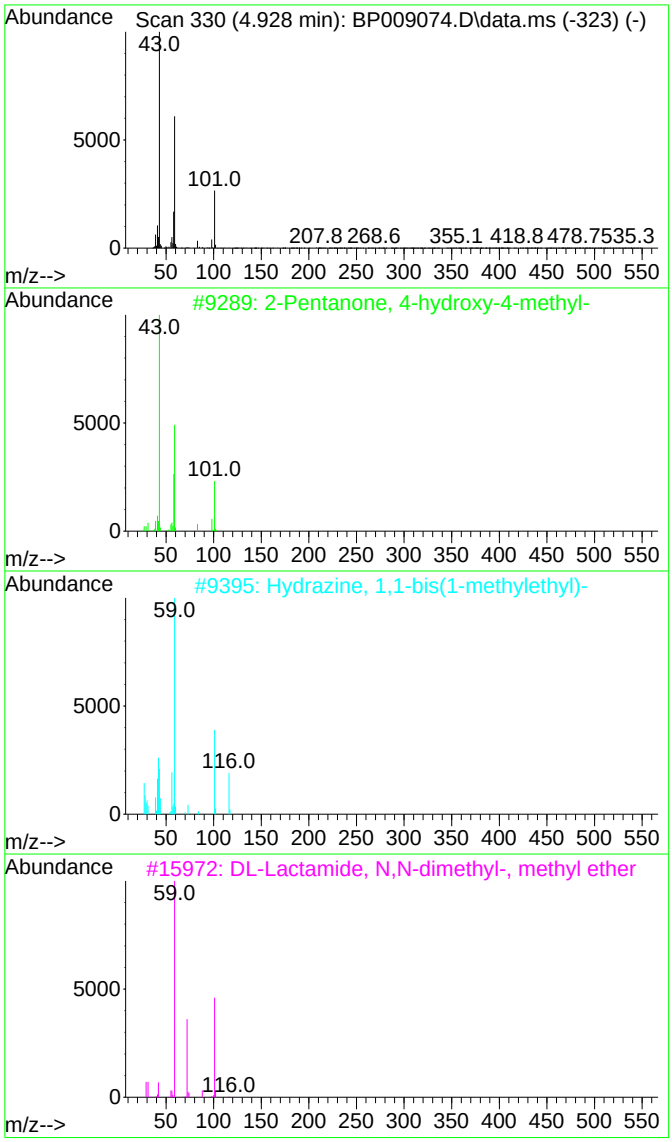
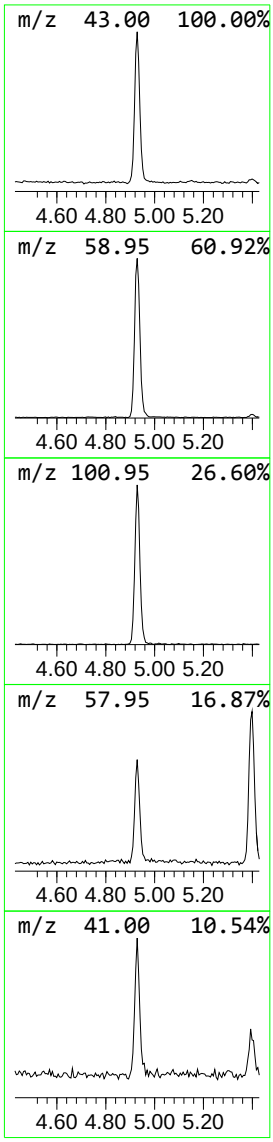
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.928	4.26 ng	228690	1,4-Dichlorobenzene-d4	7.805

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
3	DL-Lactamide, N,N-dimethyl-, met...	131	C6H13NO2	1000452-57-0	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5	2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	17





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Operator : CG/JU
Sample : N1421-01
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Instrument :
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ClientSampleId :
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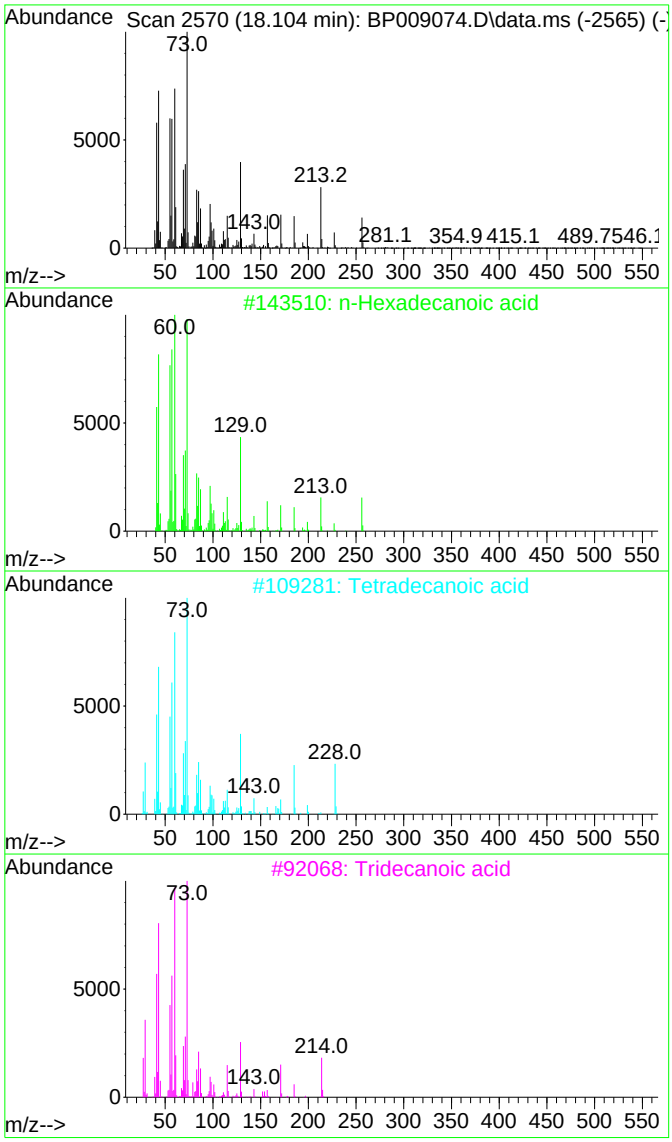
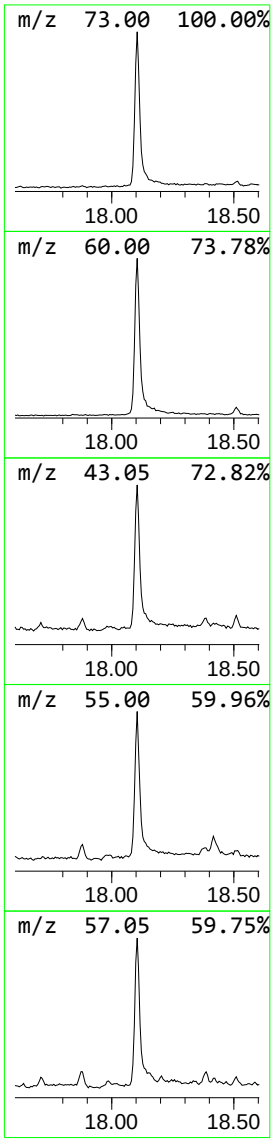
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.104	6.38 ng	1000690	Phenanthrene-d10	17.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Octadecanoic acid	284	C18H36O2	000057-11-4	87





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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
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TIC Library : C:\Database\NIST20.L
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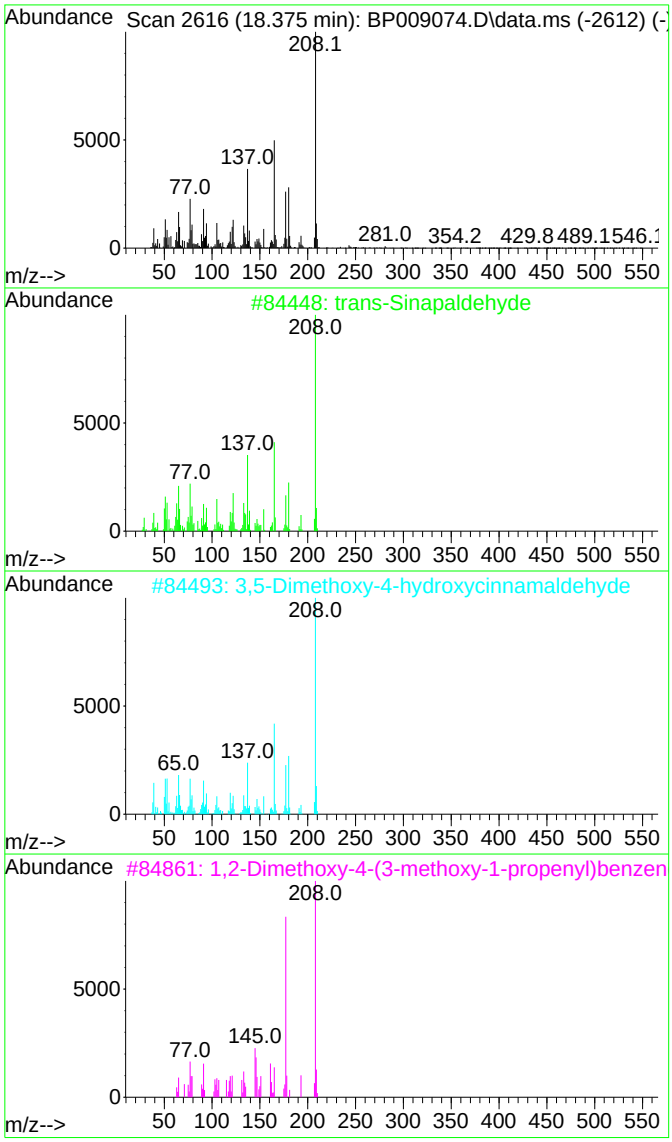
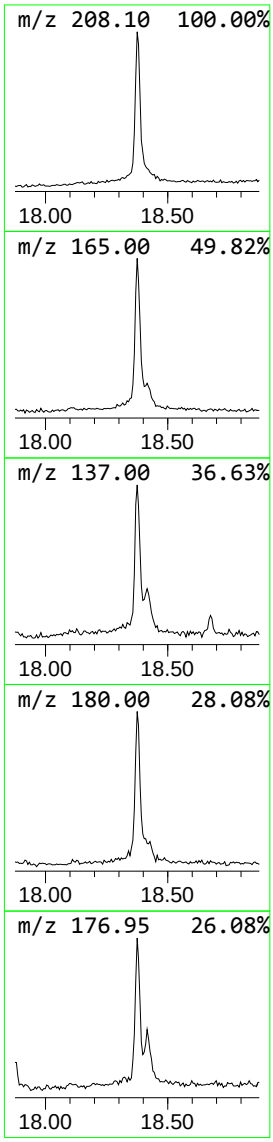
Peak Number 3 trans-Sinapaldehyde Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.375	2.08 ng	325738	Phenanthrene-d10	17.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Sinapaldehyde	208	C11H12O4	004206-58-0	97
2	3,5-Dimethoxy-4-hydroxycinnamald...	208	C11H12O4	087345-53-7	91
3	1,2-Dimethoxy-4-(3-methoxy-1-pro...	208	C12H16O3	1000313-35-0	60
4	Pyrene, 1,2,3,6,7,8-hexahydro-	208	C16H16	001732-13-4	47
5	6-Amino-2-(4-methylpiperidin-1-y...	208	C10H16N4O	1000388-65-9	46





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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.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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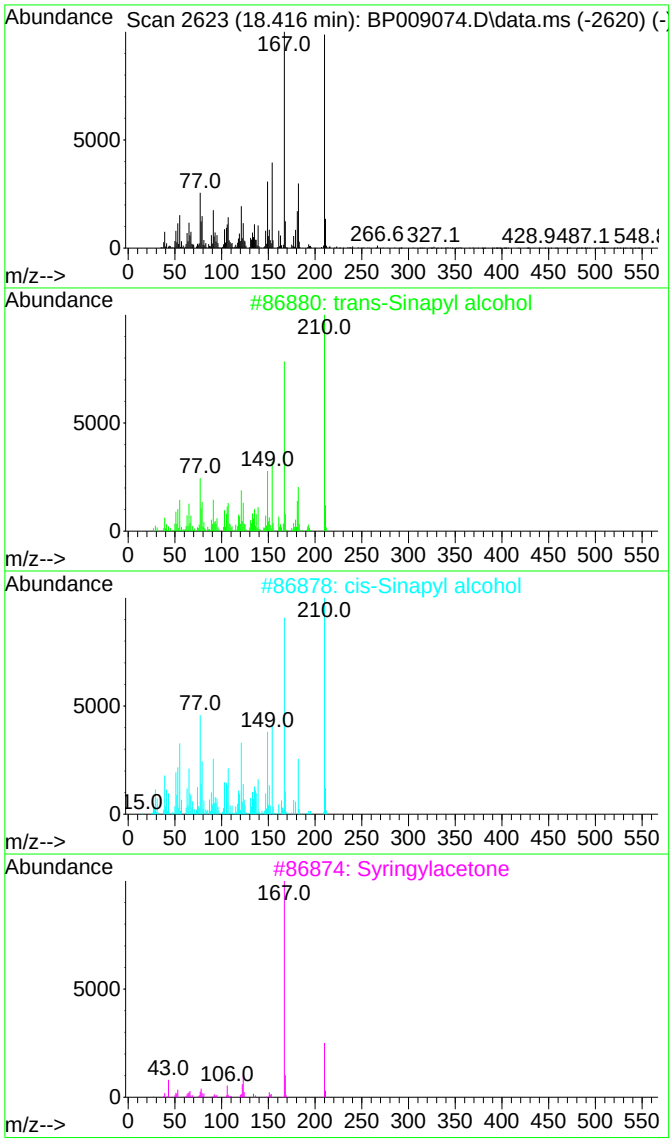
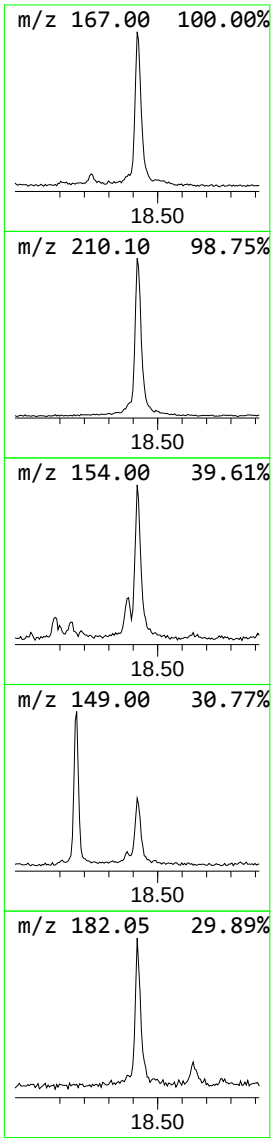
Peak Number 4 trans-Sinapyl alcohol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.416	3.12 ng	489017	Phenanthrene-d10	17.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Sinapyl alcohol	210	C11H14O4	020675-96-1	94
2	cis-Sinapyl alcohol	210	C11H14O4	104330-63-4	90
3	Syringylacetone	210	C11H14O4	019037-58-2	60
4	1-Butanone, 1-(2,4,6-trihydroxy-...	210	C11H14O4	001509-06-4	49
5	2-Methyl-2,8-diazaspiro[5.5]unde...	210	C10H14N2O3	632298-56-7	43





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Sample : N1421-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
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TIC Library : C:\Database\NIST20.L
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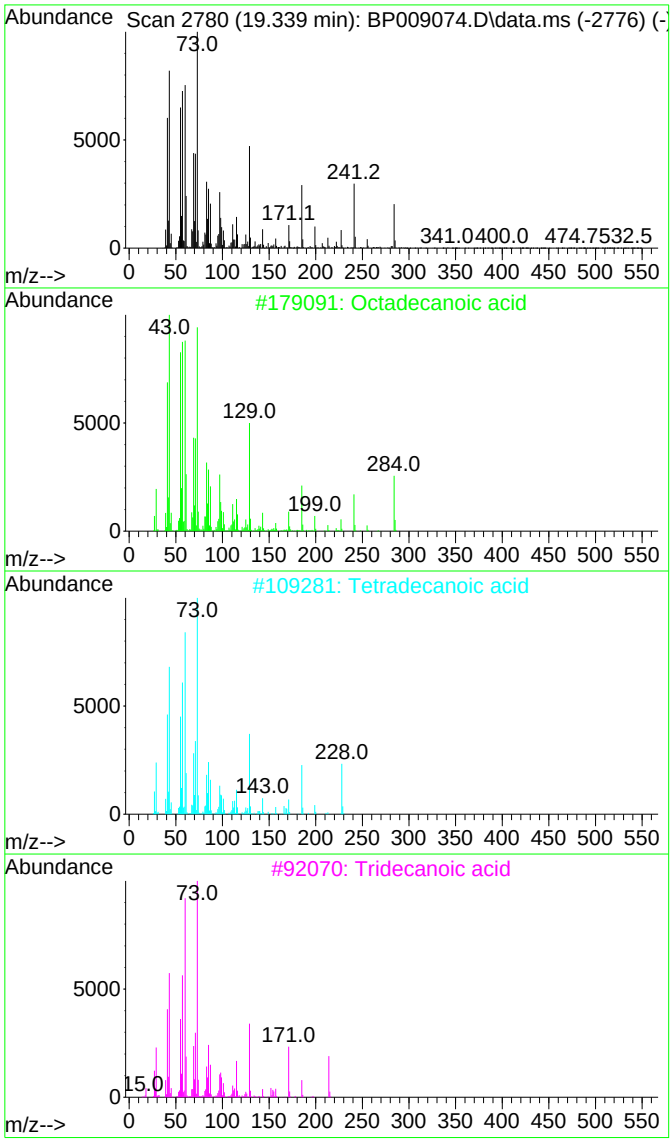
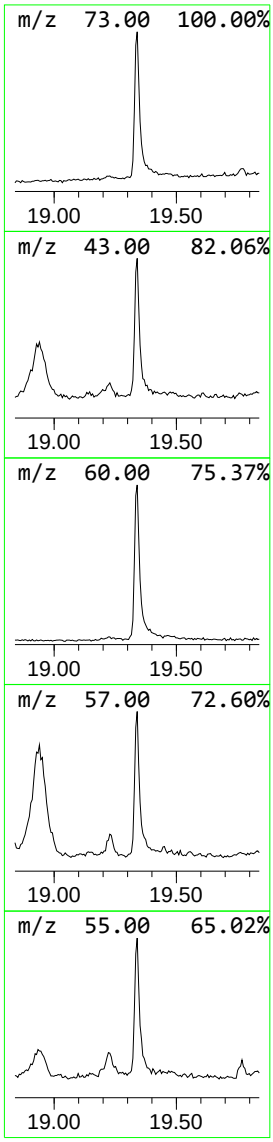
Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.339	4.04 ng	734765	Chrysene-d12	21.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
3	Tridecanoic acid	214	C13H26O2	000638-53-9	70
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	62





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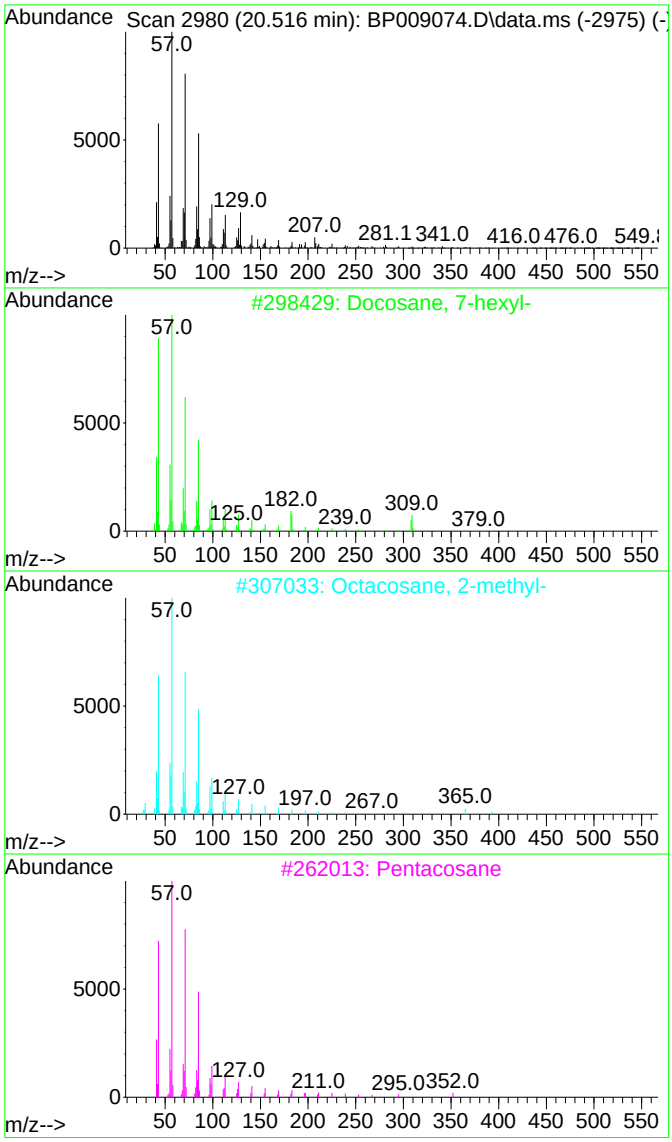
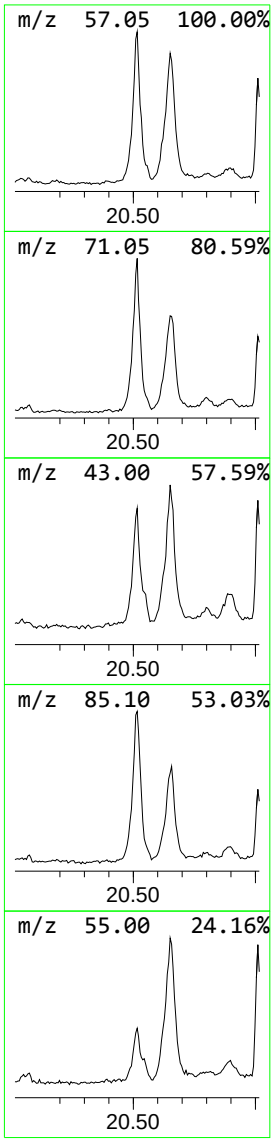
****

Peak Number 6 Docosane, 7-hexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.516	4.59 ng	834806	Chrysene-d12	21.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 7-hexyl-	394	C28H58	055373-86-9	94
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3	Pentacosane	352	C25H52	000629-99-2	91
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	91
5	Hexacosane	366	C26H54	000630-01-3	91





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TIC Library : C:\Database\NIST20.L
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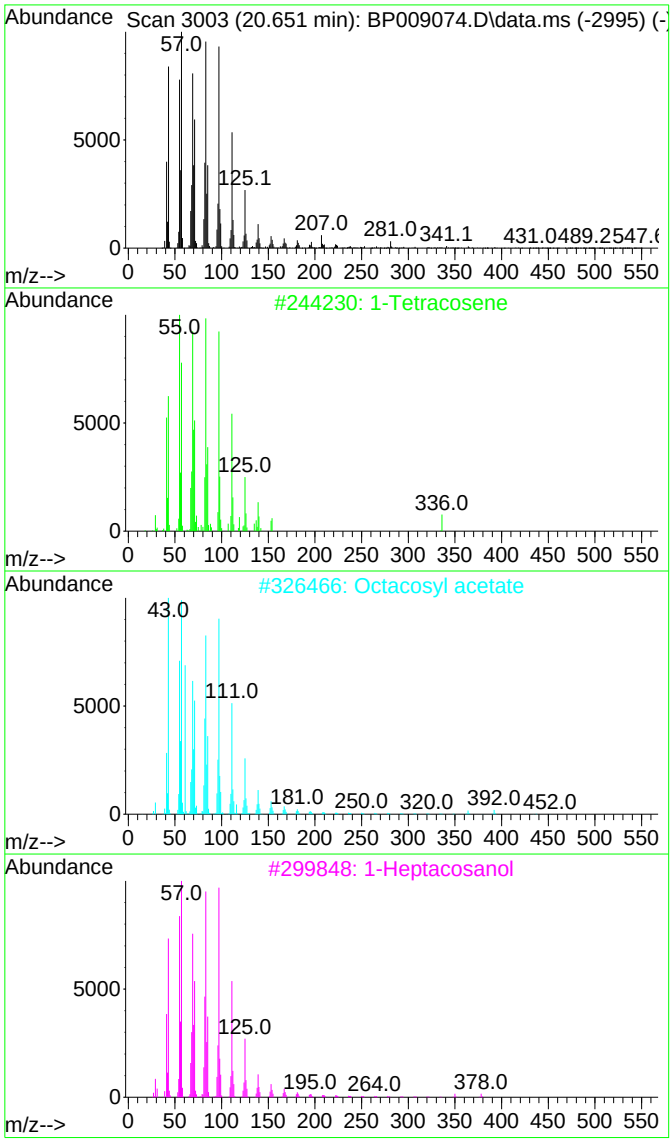
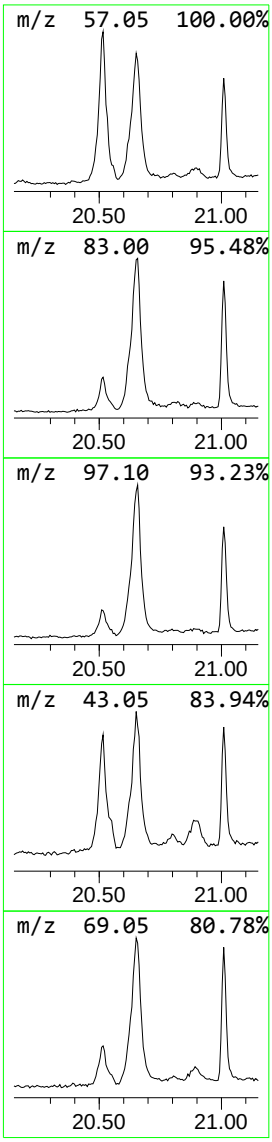
****

Peak Number 7 1-Tetracosene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.651	8.67 ng	1576340	Chrysene-d12	21.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	97
2	Octacosyl acetate	452	C30H60O2	018206-97-8	95
3	1-Heptacosanol	396	C27H56O	002004-39-9	95
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5	Nonacos-1-ene	406	C29H58	018835-35-3	94





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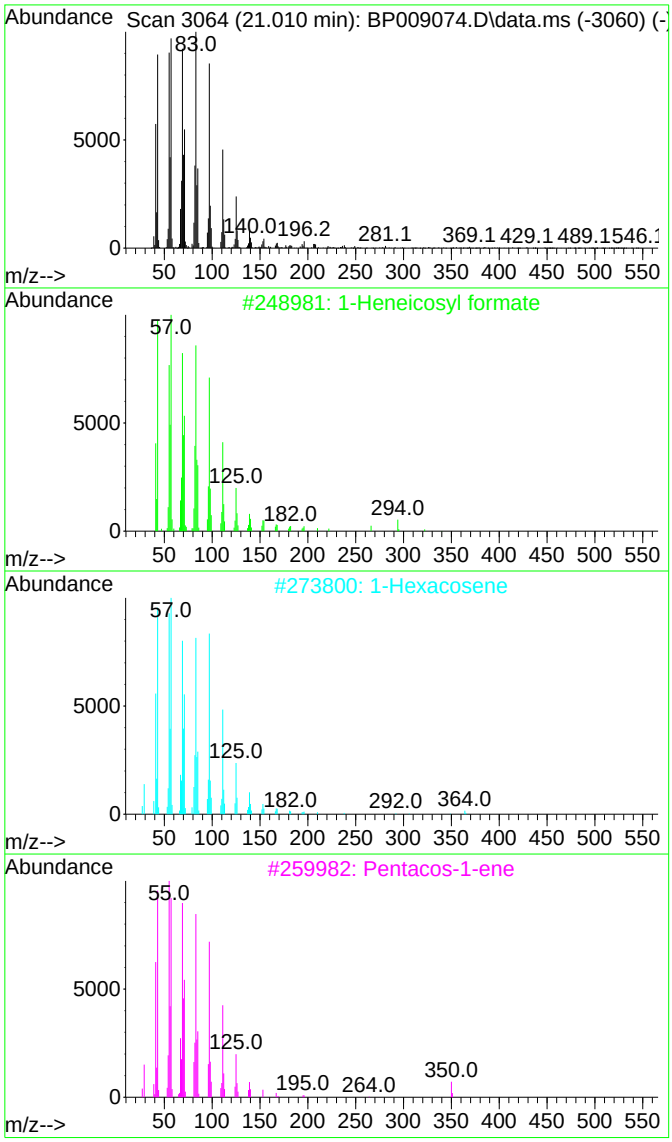
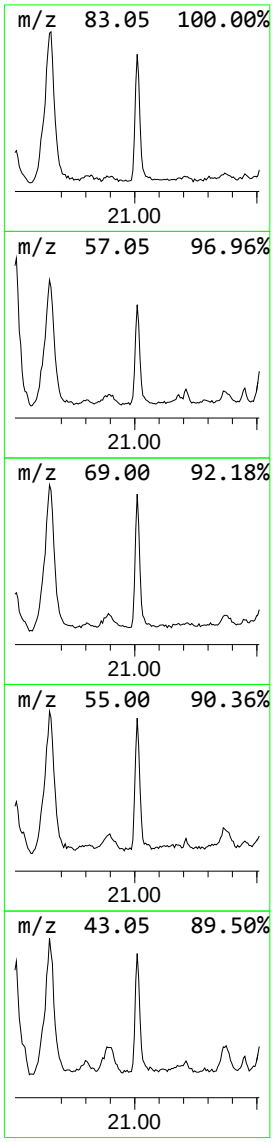
****

Peak Number 8 1-Heneicosyl formate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.010	4.14 ng	753198	Chrysene-d12	21.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	97
2	1-Hexacosene	364	C26H52	018835-33-1	94
3	Pentacos-1-ene	350	C25H50	016980-85-1	94
4	1-Tetracosene	336	C24H48	010192-32-2	94
5	1-Heptacosanol	396	C27H56O	002004-39-9	94





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Instrument :
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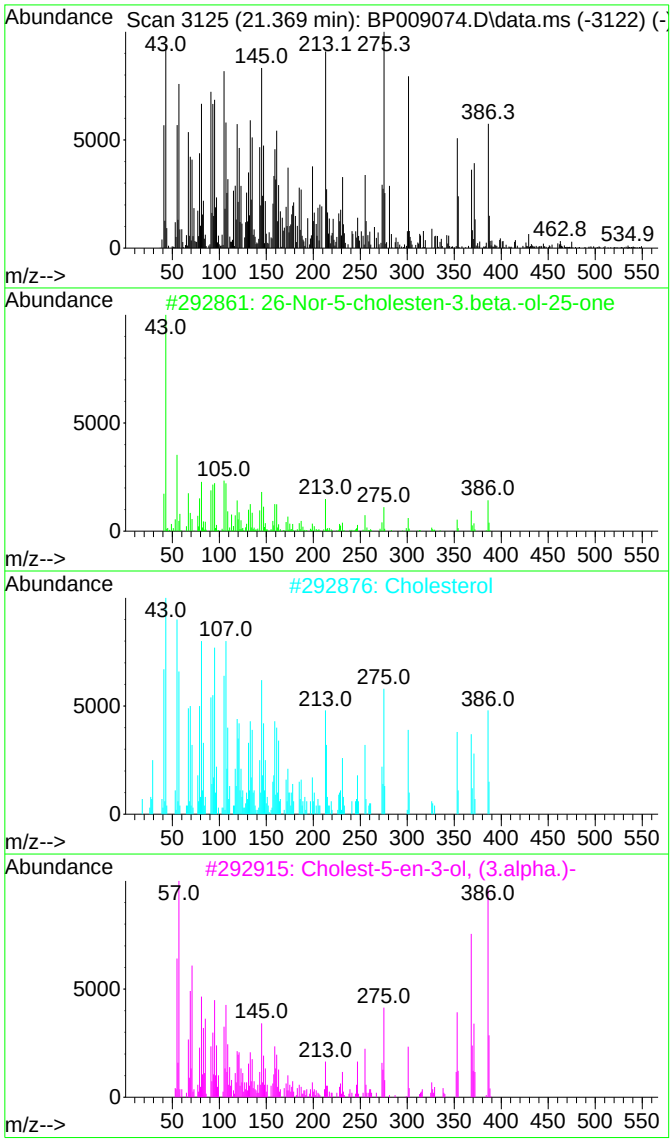
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

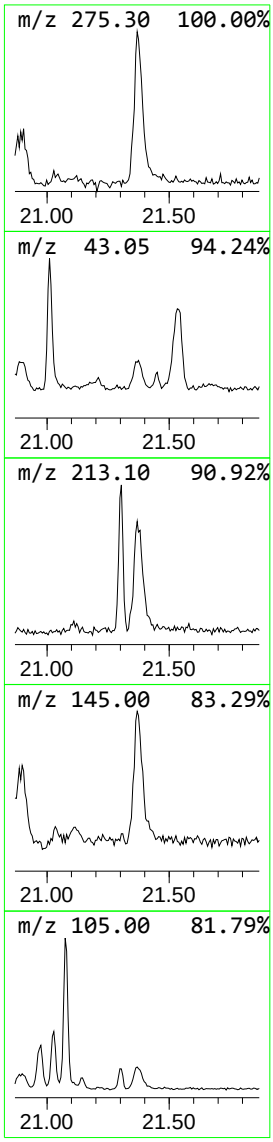
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 26-Nor-5-cholesten-3.beta.-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.369	2.21 ng	401071	Chrysene-d12	21.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	95
2	Cholesterol	386	C27H46O	000057-88-5	62
3	Cholest-5-en-3-ol, (3.alpha.)-	386	C27H46O	000474-77-1	58
4	Propanoic acid, 3,3,3-trifluoro-...	386	C17H17F3N2O5	1000362-46-1	45
5	Cholest-8-en-3-ol, (3.beta.)-	386	C27H46O	007199-91-9	44





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020922\
Data File : BP009074.D
Acq On : 09 Feb 2022 13:02
Operator : CG/JU
Sample : N1421-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

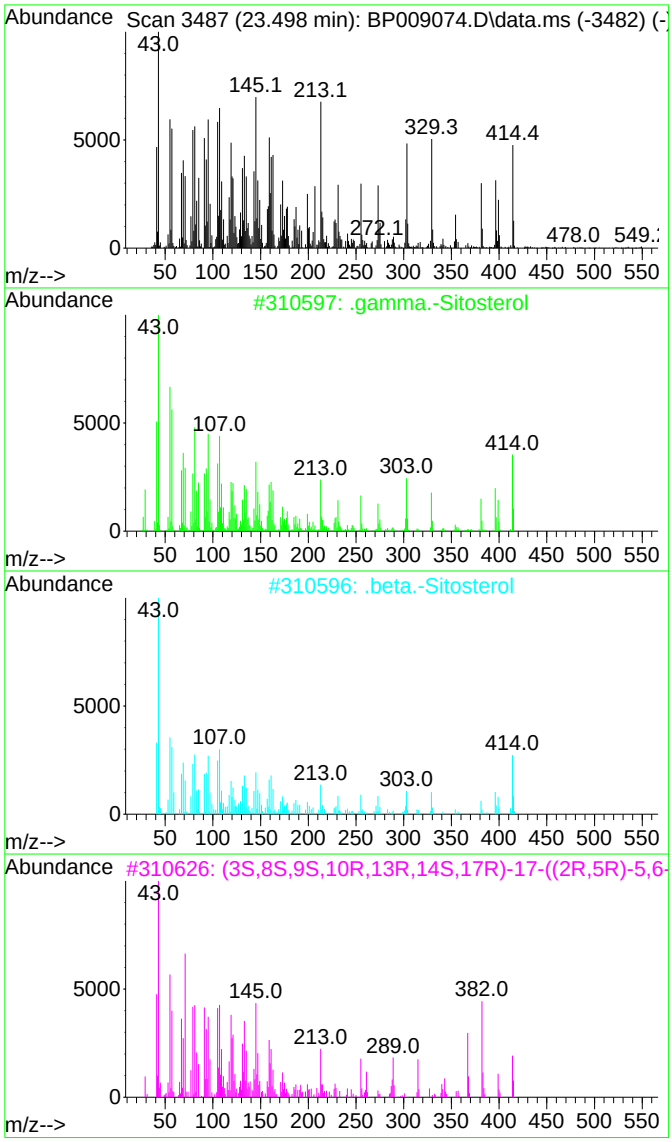
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

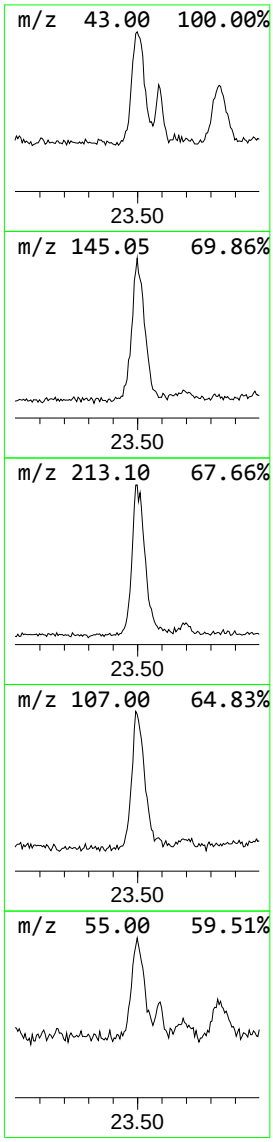
****

Peak Number 10 .gamma.-Sitosterol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.498	7.46 ng	1485600	Perylene-d12	23.704

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	90
3	(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	11
4	5.alpha.-Stigmast-9(11)-en-3.bet...	414	C29H50O	077794-81-1	10
5	cis-4-Acetoxy-trans-1-(m-methoxy...	273	C16H19NO3	1000241-10-4	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020922\
Data File : BP009074.D
Acq On : 09 Feb 2022 13:02
Operator : CG/JU
Sample : N1421-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.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-...	4.928	4.3	ng	228690	1	7.805	1072490	20.0
n-Hexadecanoic ...	18.104	6.4	ng	1000690	4	17.204	3138450	20.0
trans-Sinapalde...	18.375	2.1	ng	325738	4	17.204	3138450	20.0
trans-Sinapyl a...	18.416	3.1	ng	489017	4	17.204	3138450	20.0
Octadecanoic acid	19.339	4.0	ng	734765	5	21.304	3637390	20.0
Docosane, 7-hexyl-	20.516	4.6	ng	834806	5	21.304	3637390	20.0
1-Tetracosene	20.651	8.7	ng	1576340	5	21.304	3637390	20.0
1-Heneicosyl fo...	21.010	4.1	ng	753198	5	21.304	3637390	20.0
26-Nor-5-choles...	21.369	2.2	ng	401071	5	21.304	3637390	20.0
.gamma.-Sitosterol	23.498	7.5	ng	1485600	6	23.704	3981650	20.0