LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006538.D
Acq On : 06 Aug 2021 14:20
Operator : CG/JU
Sample : M3274-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : HD-01-080321

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-BP080321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006538.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.905	305	309	316	rVB	549447	763081	16.08%	2.051%
2	5.358	380	386	399	rVB	1794260	2519858	53.09%	6.773%
3	5.969	486	490	498	rVB	116568	169410	3.57%	0.455%
4	6.934	648	654	663	rVB	1769325	2664887	56.14%	7.163%
5	7.757	787	794	802	rVB	998557	1563297	32.93%	4.202%
6	8.910	983	990	1001	rBV	1089533	1741536	36.69%	4.681%
7	10.334	1226	1232	1241	rBV	116199	195019	4.11%	0.524%
8	10.540	1259	1267	1276	rVB	1377293	2255568	47.52%	6.063%
9	12.004	1508	1516	1523	rBV	675131	1054810	22.22%	2.835%
10	13.010	1678	1687	1696	rBV	2426200	3590343	75.64%	9.651%
11	14.234	1888	1895	1904	rBV2	38492	85018	1.79%	0.229%
12	14.381	1911	1920	1928	rBV	1818233	2758972	58.12%	7.416%
13	15.875	2167	2174	2191	rBV	1772091	2582682	54.41%	6.942%
14	17.133	2382	2388	2401	rBV	2129573	3089556	65.09%	8.305%
15	18.045	2538	2543	2552	rBV	206212	346147	7.29%	0.930%
16	19.157	2728	2732	2738	rBV	43920	65645	1.38%	0.176%
17	19.280	2750	2753	2762	rBV4	91066	174202	3.67%	0.468%
18	19.504	2788	2791	2795	rBV	65786	78571	1.66%	0.211%
19	19.710	2821	2826	2837	rBV	3843620	4746783	100.00%	12.759%
20	20.963	3036	3039	3047	rBV	288766	355084	7.48%	0.954%
21	21.233	3081	3085	3091	rBV	2487701	3107166	65.46%	8.352%
22	23.568	3475	3482	3492	rVB2	1596655	3295712	69.43%	8.859%

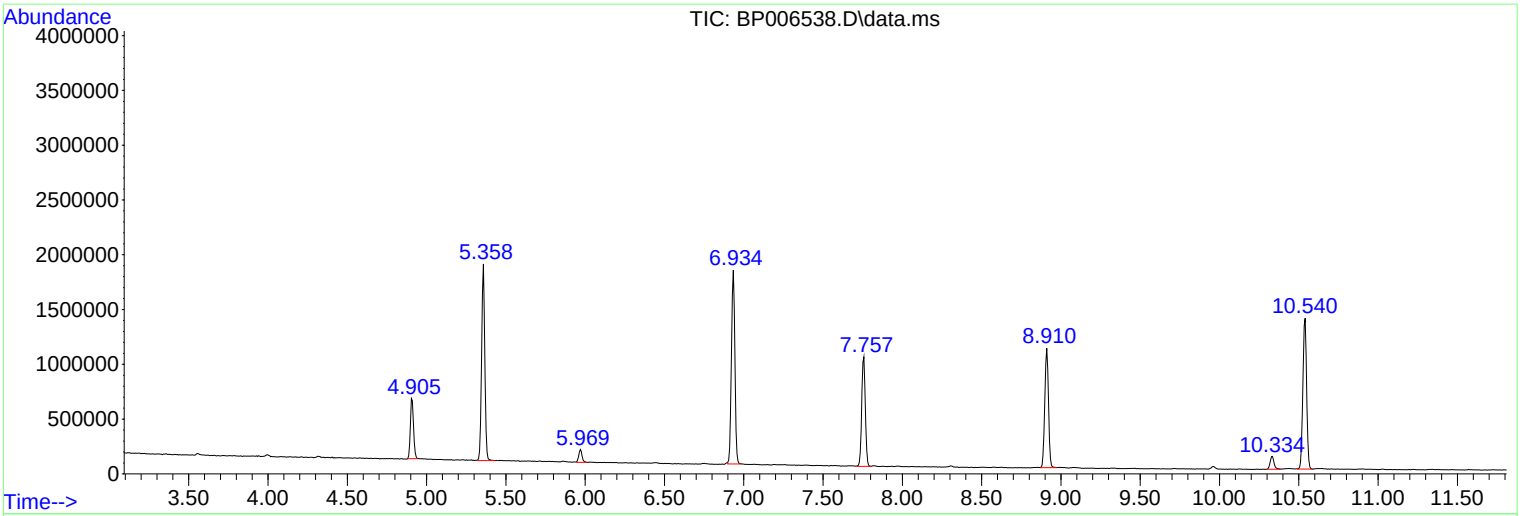
Sum of corrected areas: 37203347

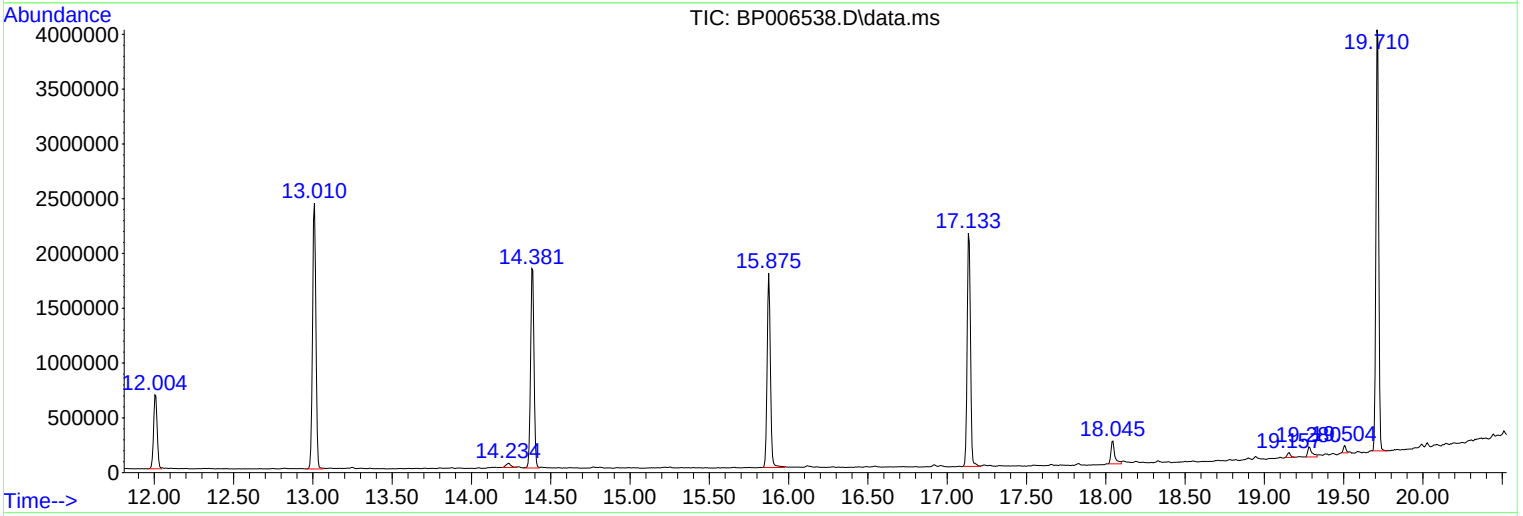
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006538.D
Acq On : 06 Aug 2021 14:20
Operator : CG/JU
Sample : M3274-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

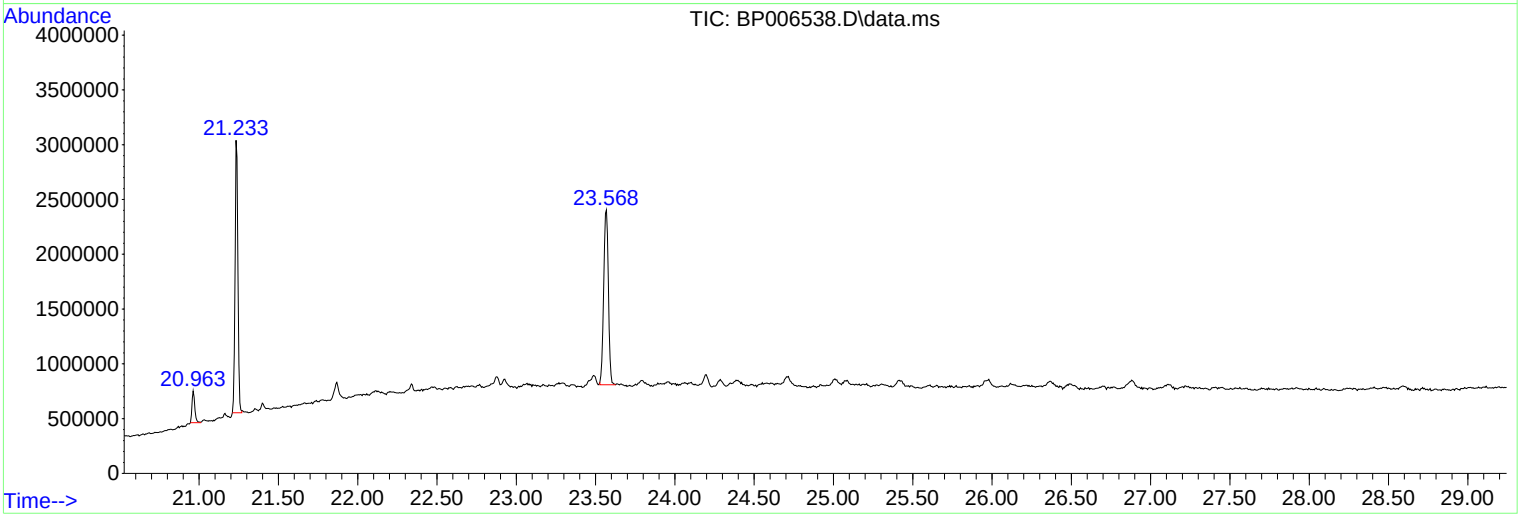
Instrument :
BNA_P
ClientSampleId :
HD-01-080321

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006538.D
Acq On : 06 Aug 2021 14:20
Operator : CG/JU
Sample : M3274-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
HD-01-080321

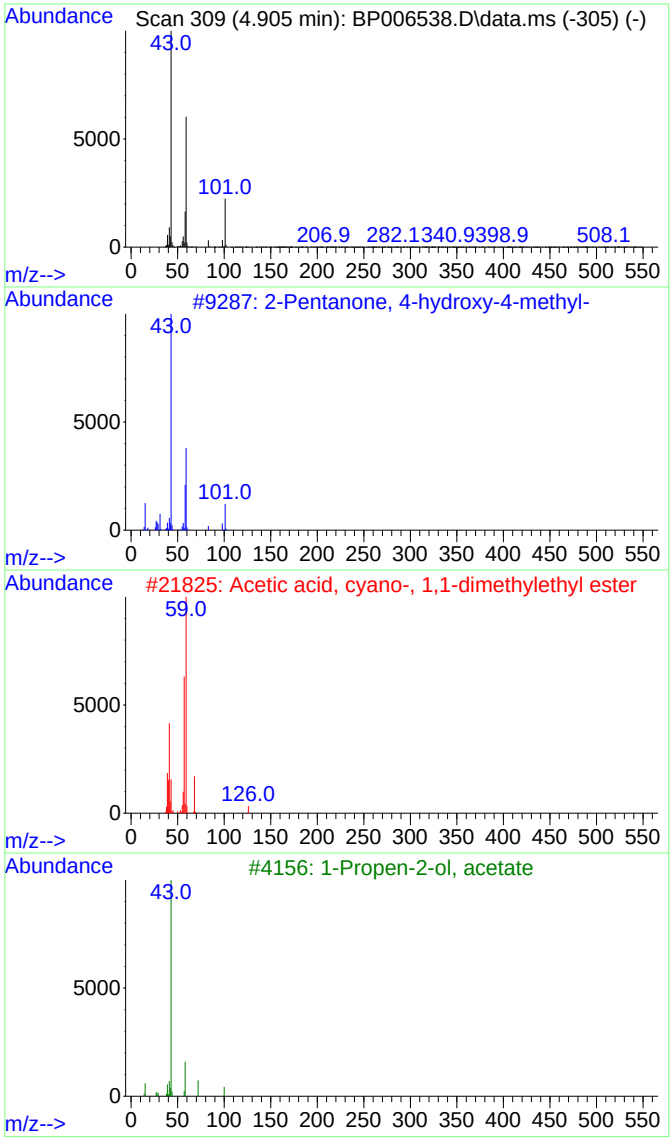
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

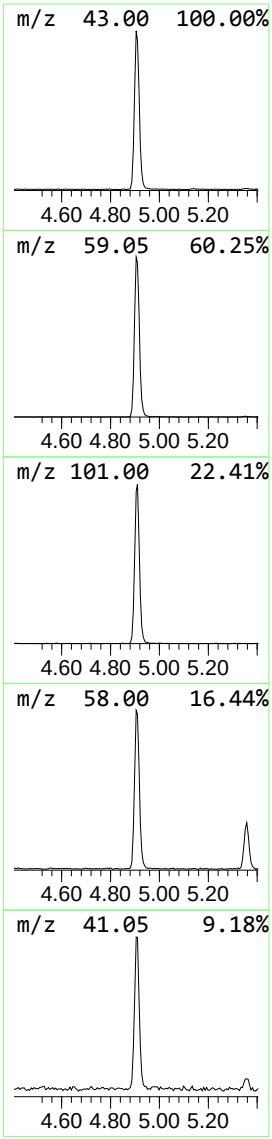
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.905	9.76 ng	763081	1,4-Dichlorobenzene-d4	7.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	4-Methoxy-1-pentene	100	C6H12O	098386-09-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006538.D
Acq On : 06 Aug 2021 14:20
Operator : CG/JU
Sample : M3274-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
HD-01-080321

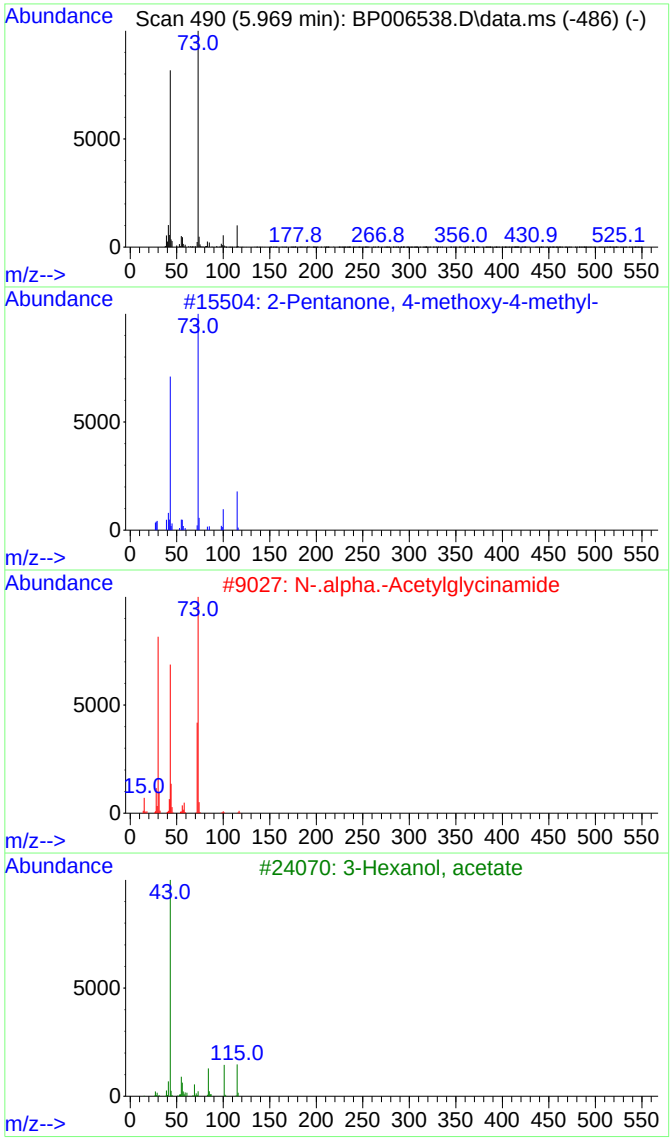
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

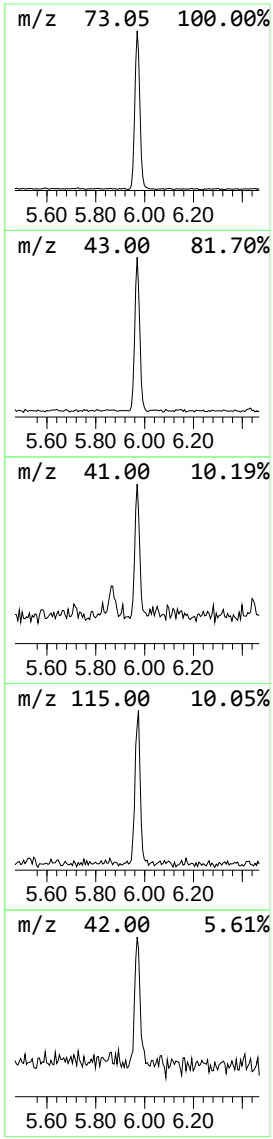
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.969	2.17 ng	169410	1,4-Dichlorobenzene-d4	7.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	40
3	3-Hexanol, acetate	144	C8H16O2	040780-64-1	25
4	4-Acetoxytridecane	242	C15H30O2	060826-30-4	25
5	Valproic Acid	144	C8H16O2	000099-66-1	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006538.D
Acq On : 06 Aug 2021 14:20
Operator : CG/JU
Sample : M3274-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : HD-01-080321

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

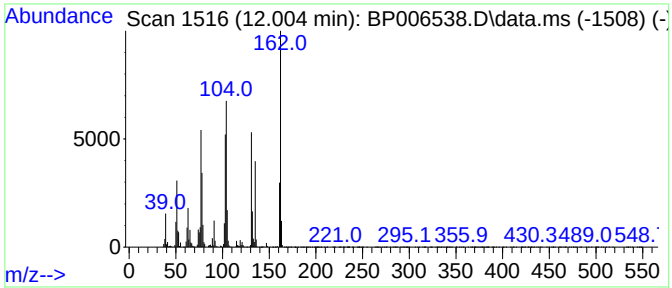
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

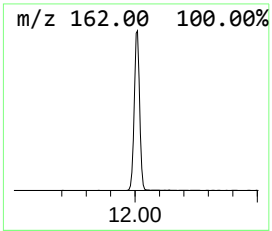
****

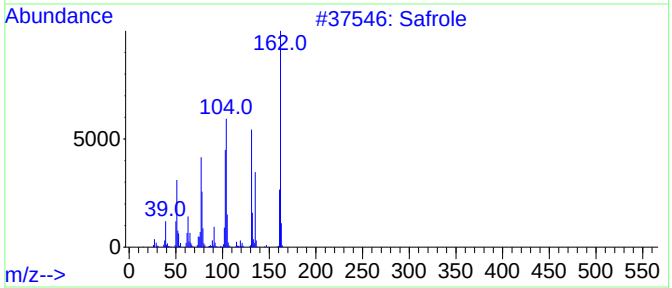
Peak Number 3 Safrole Concentration Rank 2

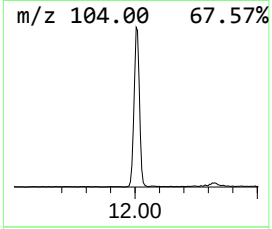
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.004	9.35 ng	1054810	Naphthalene-d8	10.540

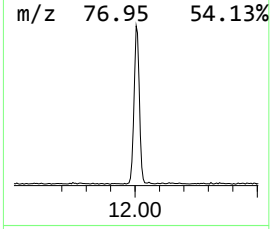
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Safrole	162	C10H10O2	000094-59-7	99
2	1,3-Benzodioxole, 5-(1-propenyl)...	162	C10H10O2	017627-76-8	98
3	Benzene, 1,2-(methylenedioxy)-4-...	162	C10H10O2	004043-71-4	98
4	1,3-Benzodioxole, 5-(1-propenyl)-	162	C10H10O2	000120-58-1	97
5	Sydnone, 3-phenyl-	162	C8H6N2O2	000120-06-9	50

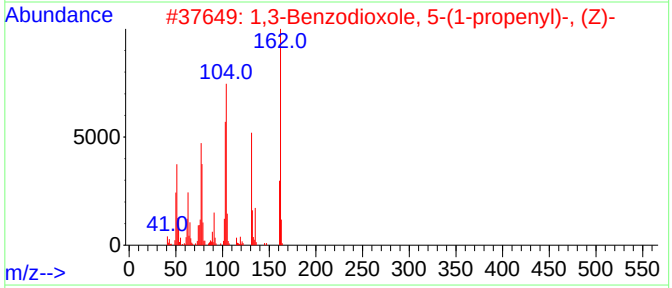


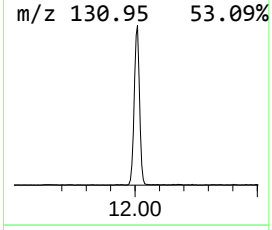


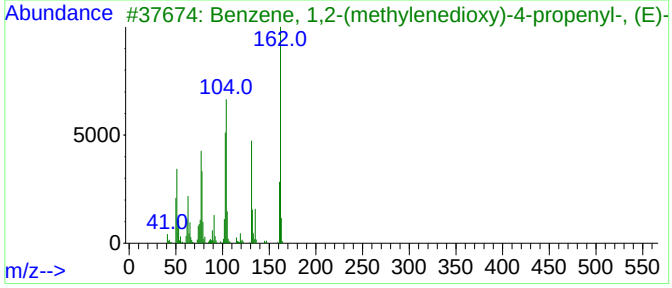


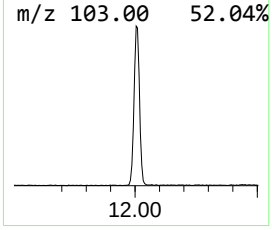












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006538.D
Acq On : 06 Aug 2021 14:20
Operator : CG/JU
Sample : M3274-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
HD-01-080321

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

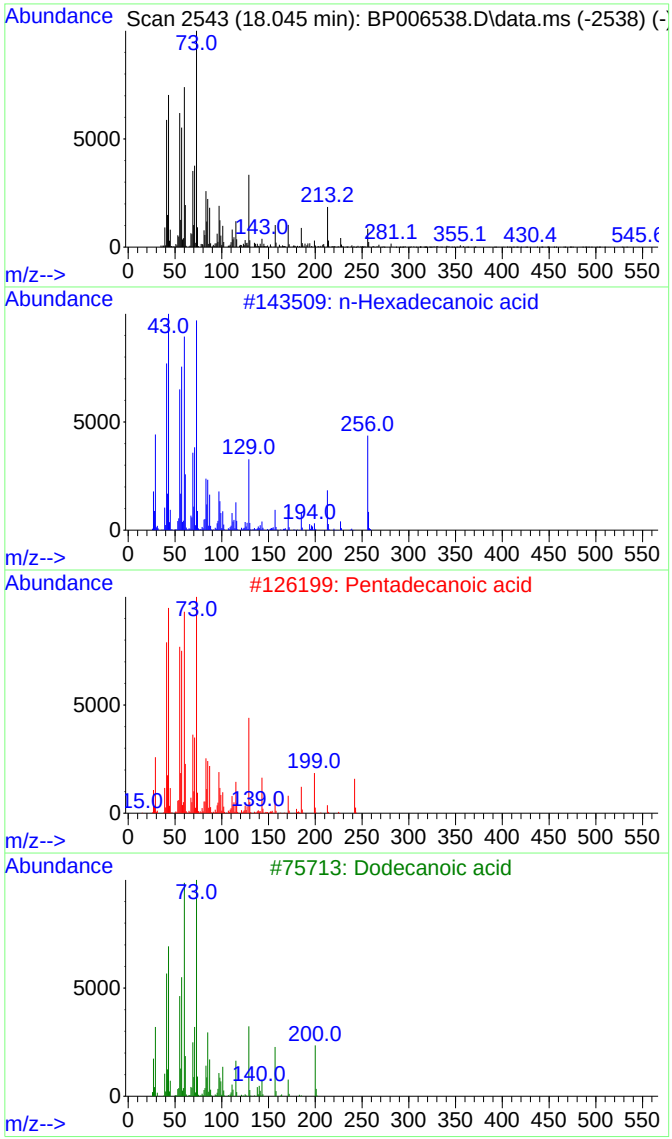
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

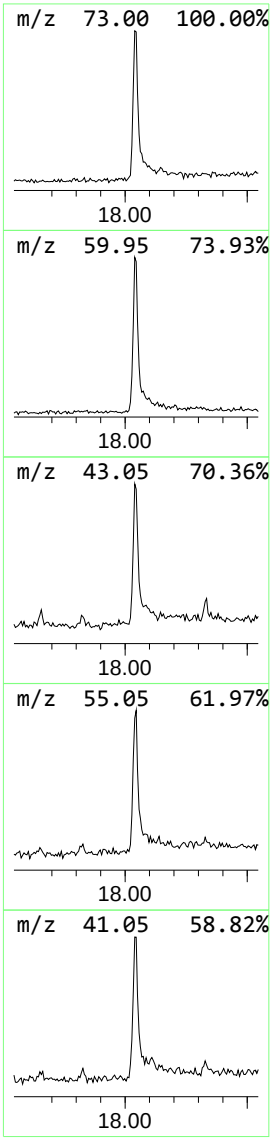
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.045	2.24 ng	346147	Phenanthrene-d10	17.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Dodecanoic acid	200	C12H24O2	000143-07-7	72
4	Tridecanoic acid	214	C13H26O2	000638-53-9	53
5	Octadecanoic acid	284	C18H36O2	000057-11-4	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006538.D
Acq On : 06 Aug 2021 14:20
Operator : CG/JU
Sample : M3274-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : HD-01-080321

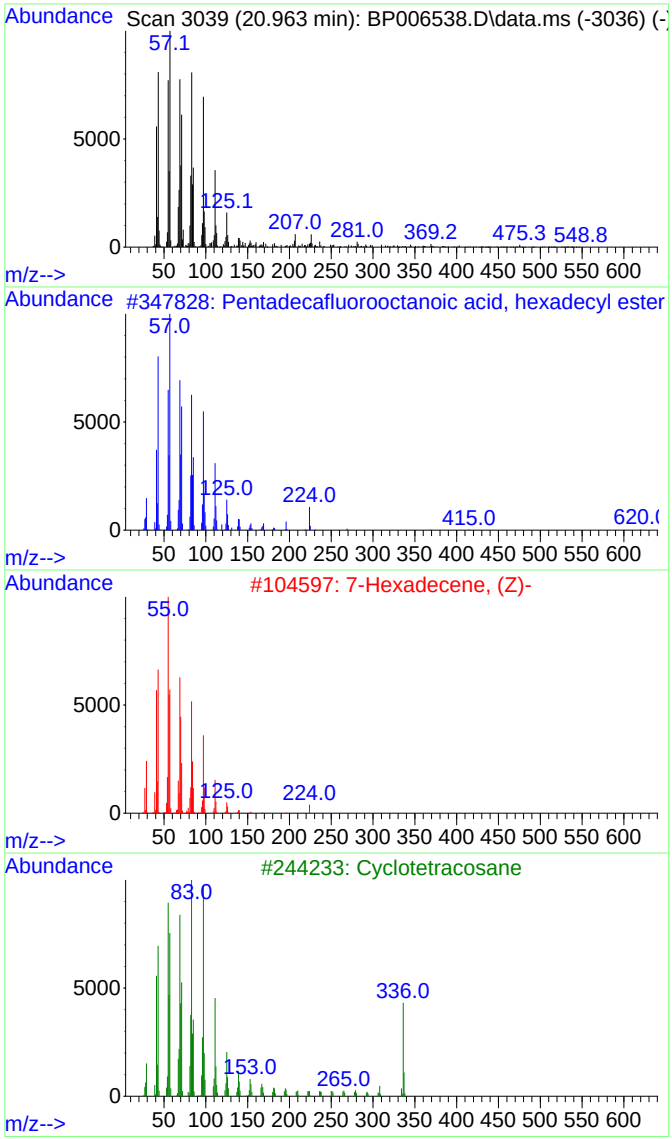
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

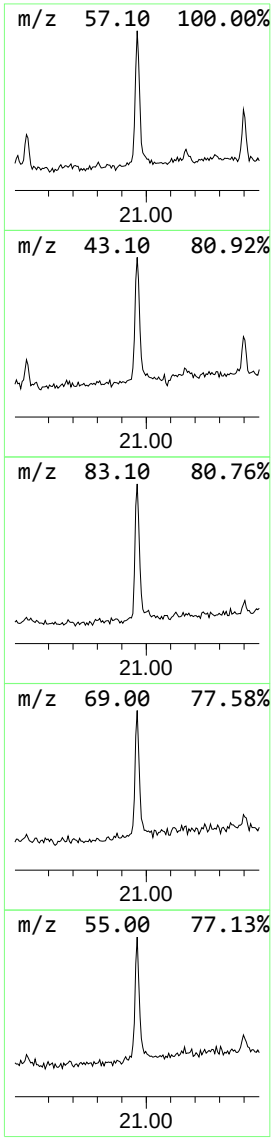
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.963	2.29 ng	355084	Chrysene-d12	21.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	94
2	7-Hexadecene, (Z)-	224	C16H32	035507-09-6	93
3	Cyclotetracosane	336	C24H48	000297-03-0	93
4	17-Pentatriacontene	491	C35H70	006971-40-0	91
5	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006538.D
Acq On : 06 Aug 2021 14:20
Operator : CG/JU
Sample : M3274-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : HD-01-080321

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.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-...	4.905	9.8	ng	763081	1	7.757	1563300	20.0
2-Pentanone, 4-...	5.969	2.2	ng	169410	1	7.757	1563300	20.0
Safrole	12.004	9.3	ng	1054810	2	10.540	2255570	20.0
n-Hexadecanoic ...	18.045	2.2	ng	346147	4	17.133	3089560	20.0
Pentadecafluoro...	20.963	2.3	ng	355084	5	21.233	3107170	20.0