LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052722\
Data File : BM035294.D
Acq On : 27 May 2022 18:11
Operator : CG/JU
Sample : N2930-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P005-SS003-0612-01

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_M\Methods\8270-BM052722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM035294.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.993	316	324	335	rBV2	43183	75057	1.63%	0.241%
2	5.387	386	391	397	rBV	91329	130557	2.83%	0.420%
3	5.457	397	403	423	rVB	1681272	2431532	52.78%	7.814%
4	5.863	465	472	481	rBV	59584	97903	2.13%	0.315%
5	6.369	552	558	564	rVB	39701	58164	1.26%	0.187%
6	7.051	665	674	692	rBV	1526294	2483112	53.90%	7.980%
7	7.875	807	814	822	rBV	499785	767405	16.66%	2.466%
8	9.034	1003	1011	1022	rBV	983683	1625981	35.29%	5.225%
9	10.675	1281	1290	1305	rVB	578286	985352	21.39%	3.167%
10	13.139	1701	1709	1722	rBV	2507582	3543937	76.93%	11.389%
11	13.398	1748	1753	1760	rVB2	114011	163512	3.55%	0.525%
12	13.845	1821	1829	1834	rBV3	34460	53942	1.17%	0.173%
13	14.363	1911	1917	1925	rBV5	22444	51013	1.11%	0.164%
14	14.510	1936	1942	1951	rBV	820866	1232836	26.76%	3.962%
15	15.998	2189	2195	2203	rBV	1768537	2506184	54.40%	8.054%
16	16.862	2336	2342	2347	rBV	62480	83018	1.80%	0.267%
17	17.256	2400	2409	2415	rBV	973106	1364990	29.63%	4.387%
18	17.939	2520	2525	2529	rVB	56511	68600	1.49%	0.220%
19	18.162	2557	2563	2571	rBV	668046	976674	21.20%	3.139%
20	18.227	2571	2574	2581	rVB	50494	83741	1.82%	0.269%
21	19.109	2720	2724	2728	rVB	206446	217256	4.72%	0.698%
22	19.239	2743	2746	2750	rBV	51544	62597	1.36%	0.201%
23	19.292	2750	2755	2756	rBV3	53632	67840	1.47%	0.218%
24	19.439	2775	2780	2797	rBV	641911	1014529	22.02%	3.260%
25	19.698	2821	2824	2829	rVB	64004	86343	1.87%	0.277%
26	19.880	2849	2855	2862	rBV	3868498	4606875	100.00%	14.805%
27	20.168	2901	2904	2907	rBV3	38207	49290	1.07%	0.158%
28	20.439	2948	2950	2955	rVB4	51693	63867	1.39%	0.205%
29	21.139	3065	3069	3071	rBV	313011	461790	10.02%	1.484%
30	21.356	3102	3106	3110	rBV	646515	699962	15.19%	2.249%
31	21.433	3114	3119	3128	rBV	1364847	1961009	42.57%	6.302%
32	21.609	3145	3149	3154	rVB	296935	379399	8.24%	1.219%
33	21.662	3154	3158	3162	rBV	429535	511734	11.11%	1.645%
34	21.709	3163	3166	3168	rVV	121584	137145	2.98%	0.441%
35	21.739	3169	3171	3175	rVB	134240	137305	2.98%	0.441%
36	23.803	3516	3522	3533	rVB2	968652	1876348	40.73%	6.030%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052722\
Data File : BM035294.D
Acq On : 27 May 2022 18:11
Operator : CG/JU
Sample : N2930-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P005-SS003-0612-01

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_M\Methods\8270-BM052722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

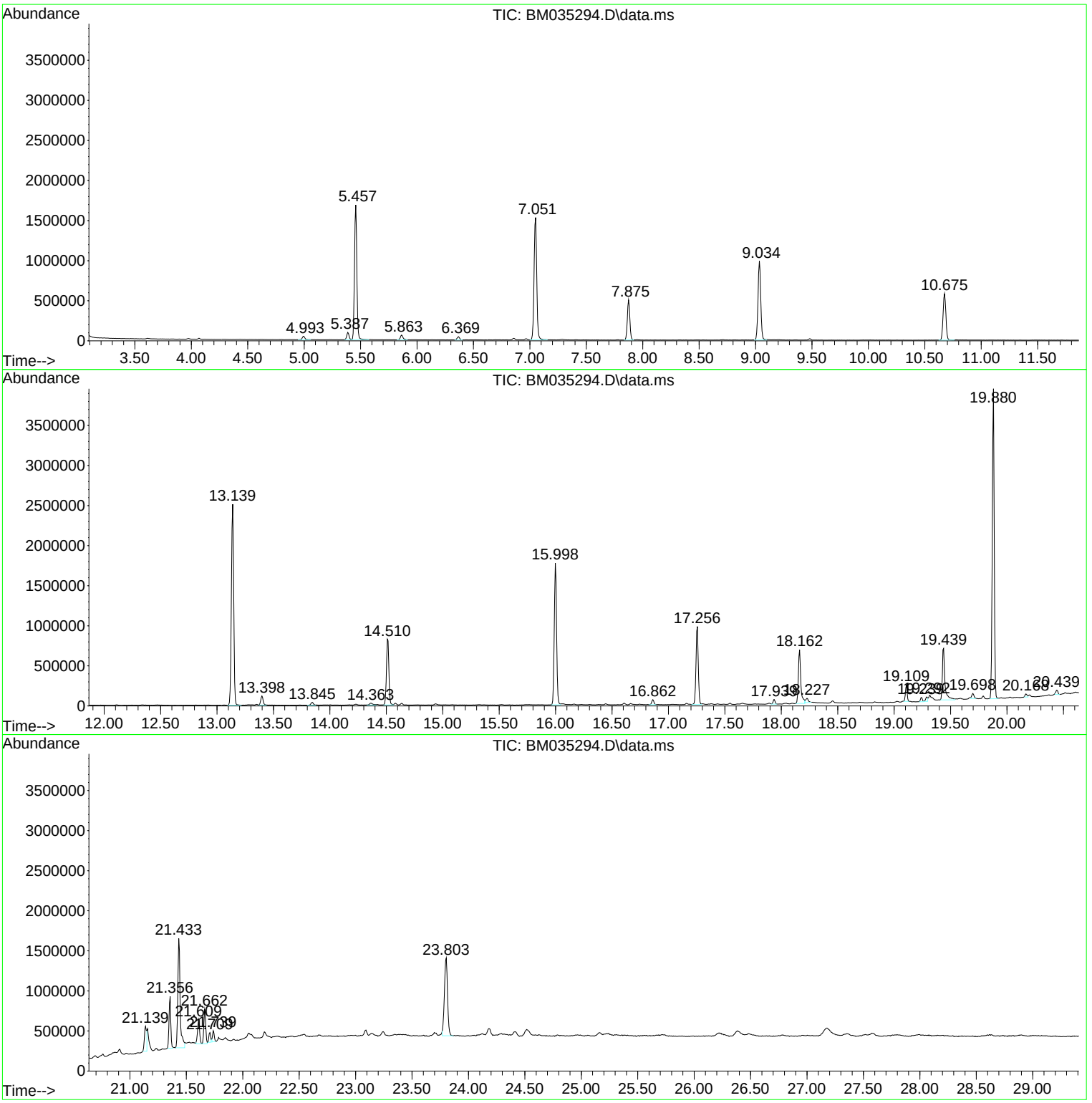
Sum of corrected areas: 31116799

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052722\
Data File : BM035294.D
Acq On : 27 May 2022 18:11
Operator : CG/JU
Sample : N2930-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P005-SS003-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.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_M\Data\BM052722\
Data File : BM035294.D
Acq On : 27 May 2022 18:11
Operator : CG/JU
Sample : N2930-08
Misc :
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Instrument :
BNA_M
ClientSampleId :
P005-SS003-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

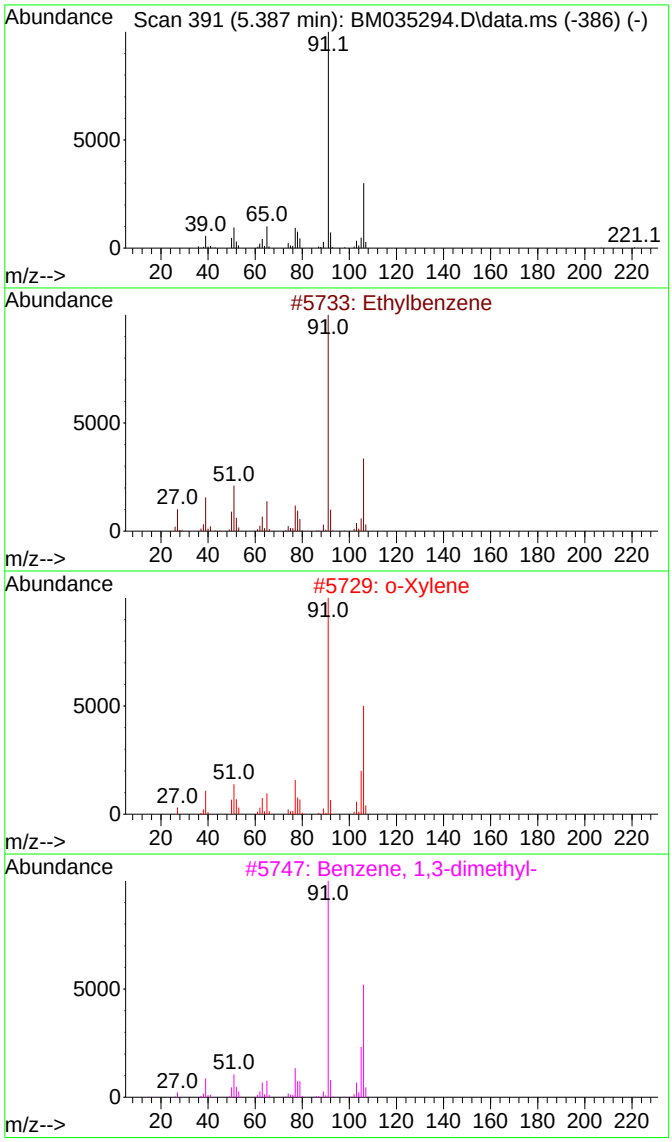
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

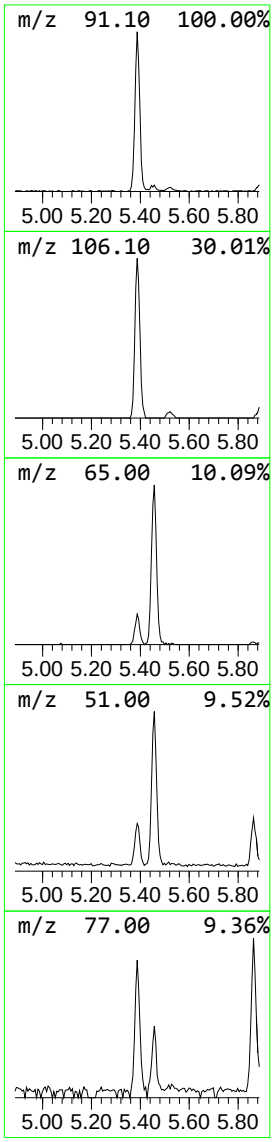
****

Peak Number 1 Ethylbenzene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.387	3.40 ng	130557	1,4-Dichlorobenzene-d4	7.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethylbenzene	106	C8H10	000100-41-4	91
2	o-Xylene	106	C8H10	000095-47-6	81
3	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	76
4	p-Xylene	106	C8H10	000106-42-3	74
5	1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052722\
Data File : BM035294.D
Acq On : 27 May 2022 18:11
Operator : CG/JU
Sample : N2930-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P005-SS003-0612-01

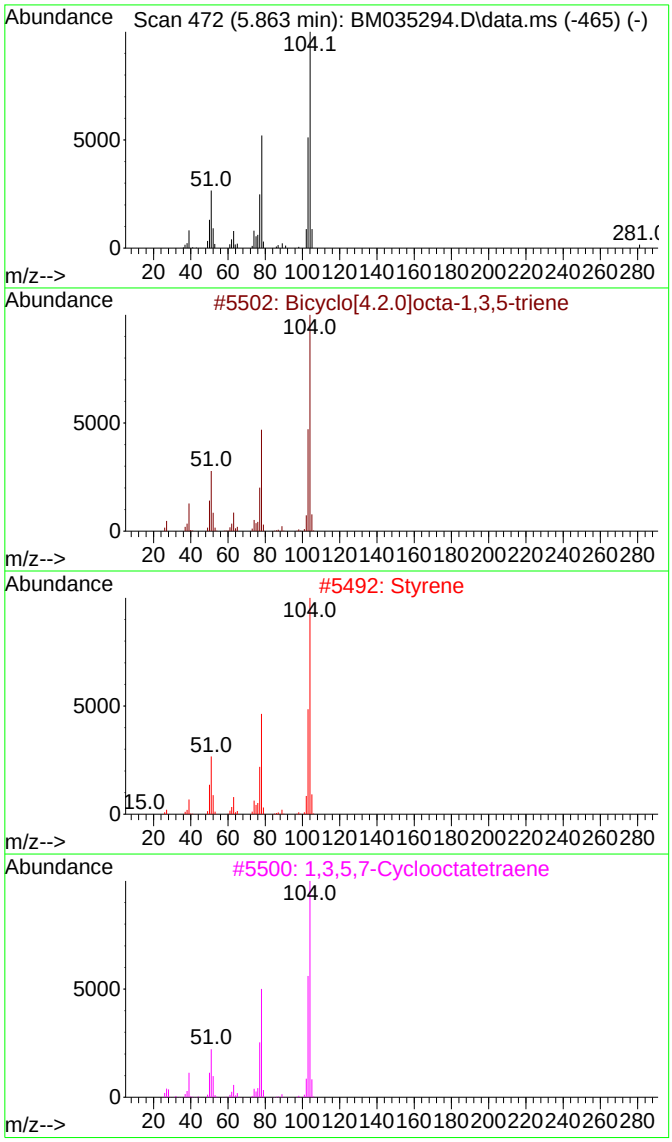
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

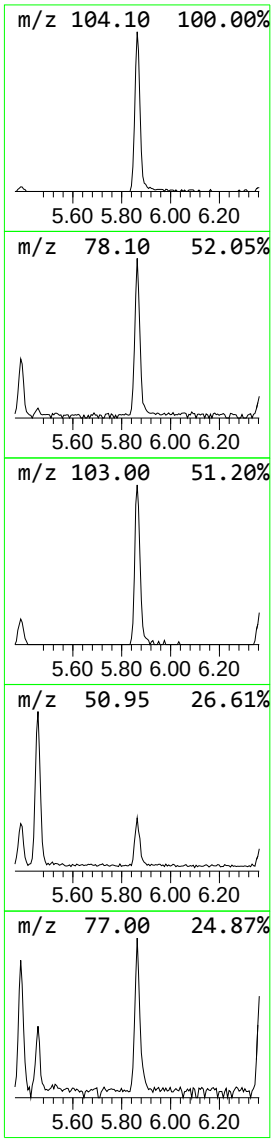
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Bicyclo[4.2.0]octa-1,3,5-tr... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.863	2.55 ng	97903	1,4-Dichlorobenzene-d4	7.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[4.2.0]octa-1,3,5-triene	104	C8H8	000694-87-1	96
2	Styrene	104	C8H8	000100-42-5	96
3	1,3,5,7-Cyclooctatetraene	104	C8H8	000629-20-9	95
4	Benzeneethanamine, N-[(4-hydroxy...	269	C17H19NO2	106827-59-2	64
5	[2.2]Paracyclophane	208	C16H16	001633-22-3	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052722\
Data File : BM035294.D
Acq On : 27 May 2022 18:11
Operator : CG/JU
Sample : N2930-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P005-SS003-0612-01

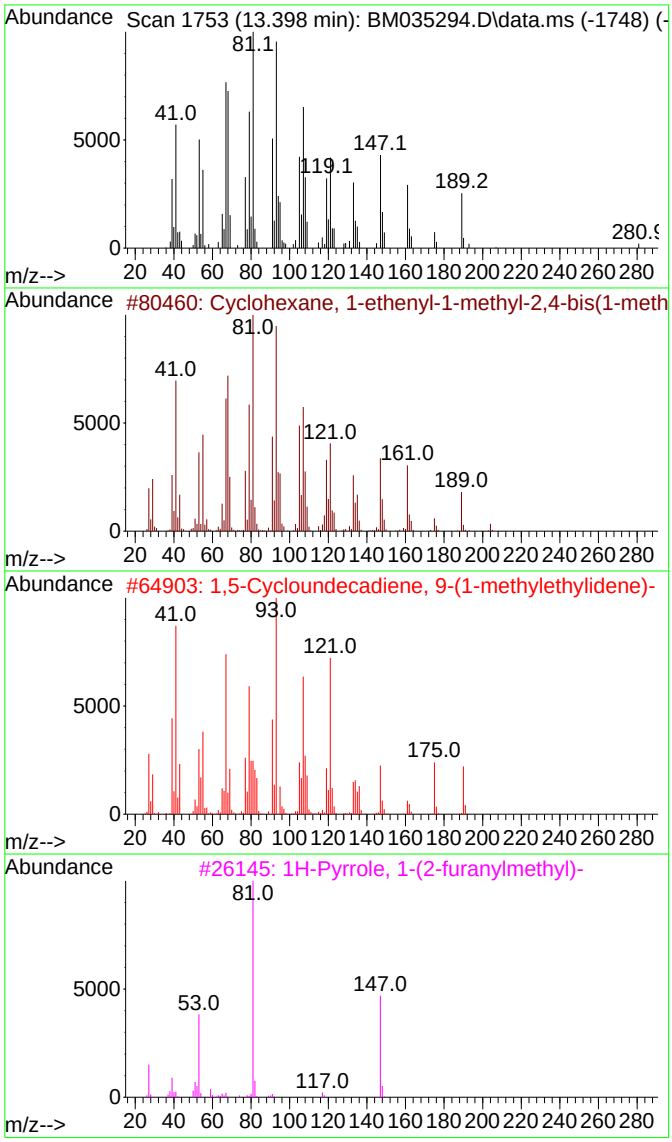
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

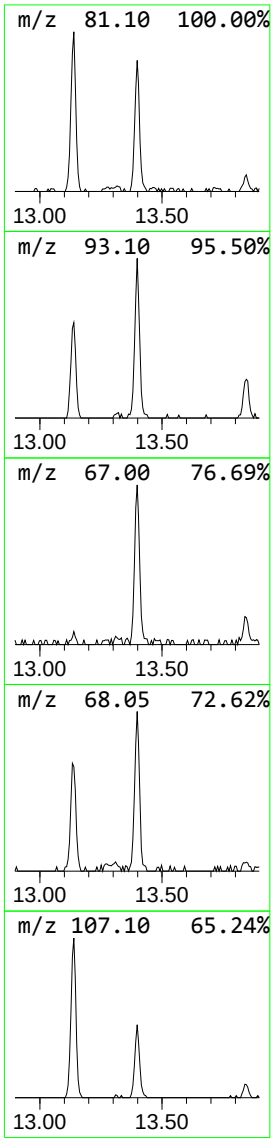
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclohexane, 1-ethenyl-1-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.398	2.65 ng	163512	Acenaphthene-d10	14.510

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethenyl-1-methyl-...	204	C15H24	000515-13-9	58
2	1,5-Cycloundecadiene, 9-(1-methy...	190	C14H22	062338-55-0	50
3	1H-Pyrrole, 1-(2-furanylmethyl)-	147	C9H9NO	001438-94-4	43
4	2,6,11-Dodecatrienal, 2,6-dimeth...	218	C15H22O	060066-88-8	43
5	Cyclohexanemethanol, 4-methylene-	126	C8H14O	001004-24-6	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052722\
Data File : BM035294.D
Acq On : 27 May 2022 18:11
Operator : CG/JU
Sample : N2930-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P005-SS003-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

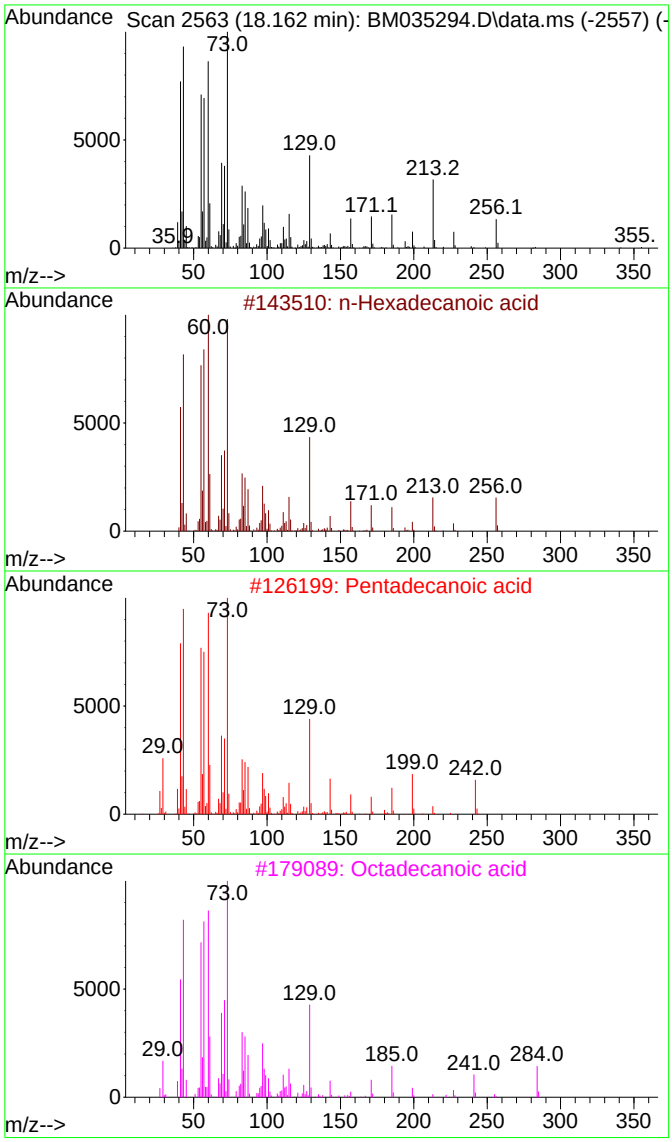
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

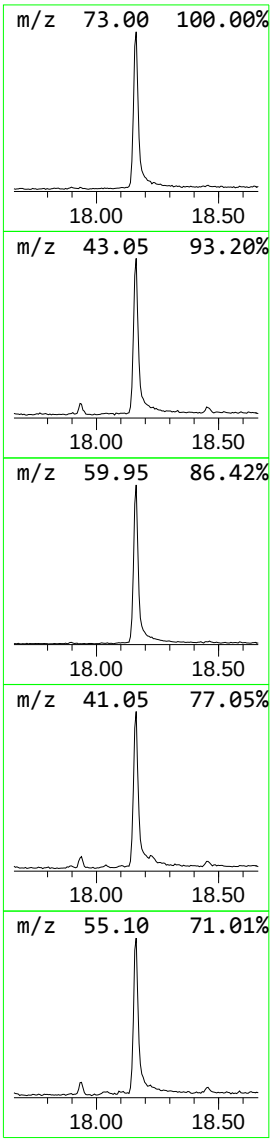
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.162	14.31 ng	976674	Phenanthrene-d10	17.256

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	91
3	Octadecanoic acid	284	C18H36O2	000057-11-4	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	87
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052722\
Data File : BM035294.D
Acq On : 27 May 2022 18:11
Operator : CG/JU
Sample : N2930-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P005-SS003-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

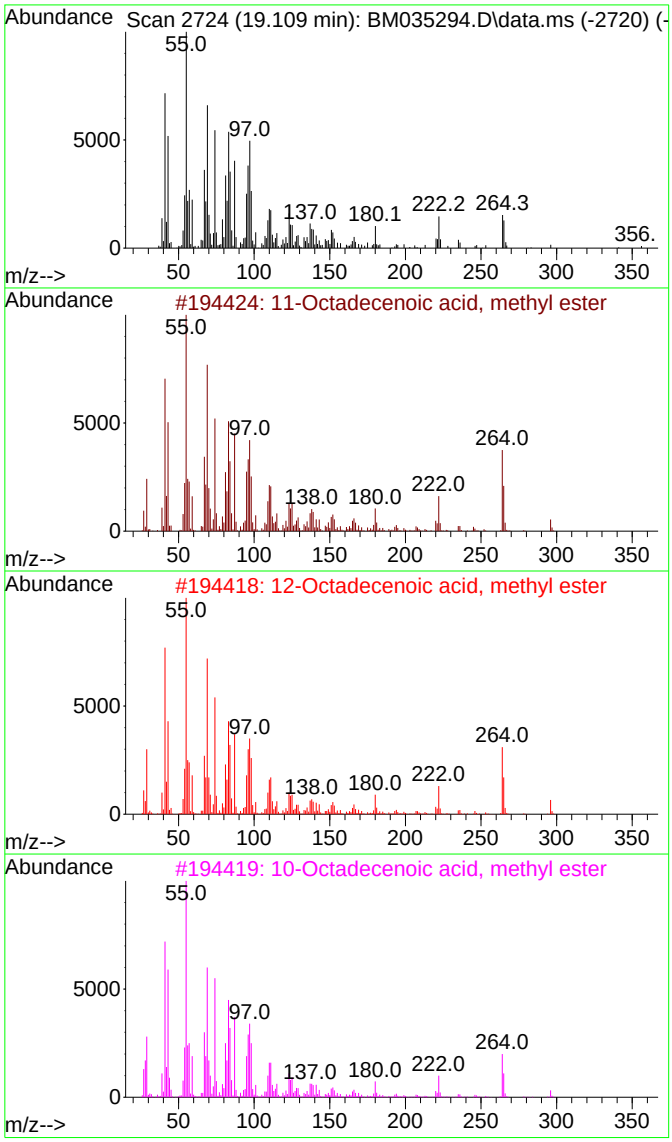
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

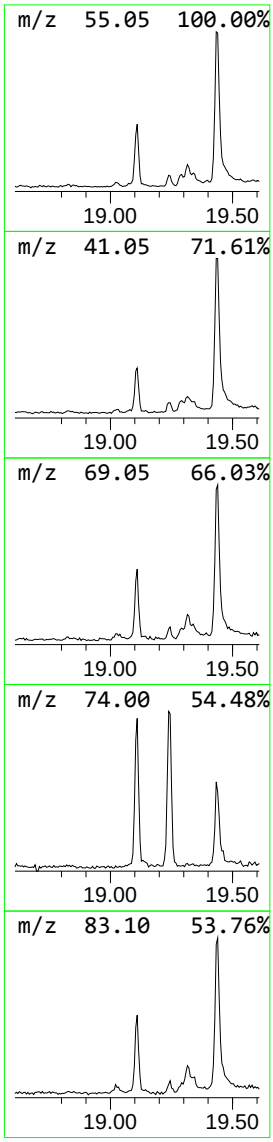
****

Peak Number 5 11-Octadecenoic acid, methy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.109	3.18 ng	217256	Phenanthrene-d10	17.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99
2	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
3	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
4	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
5	6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	99





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052722\
Data File : BM035294.D
Acq On : 27 May 2022 18:11
Operator : CG/JU
Sample : N2930-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P005-SS003-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

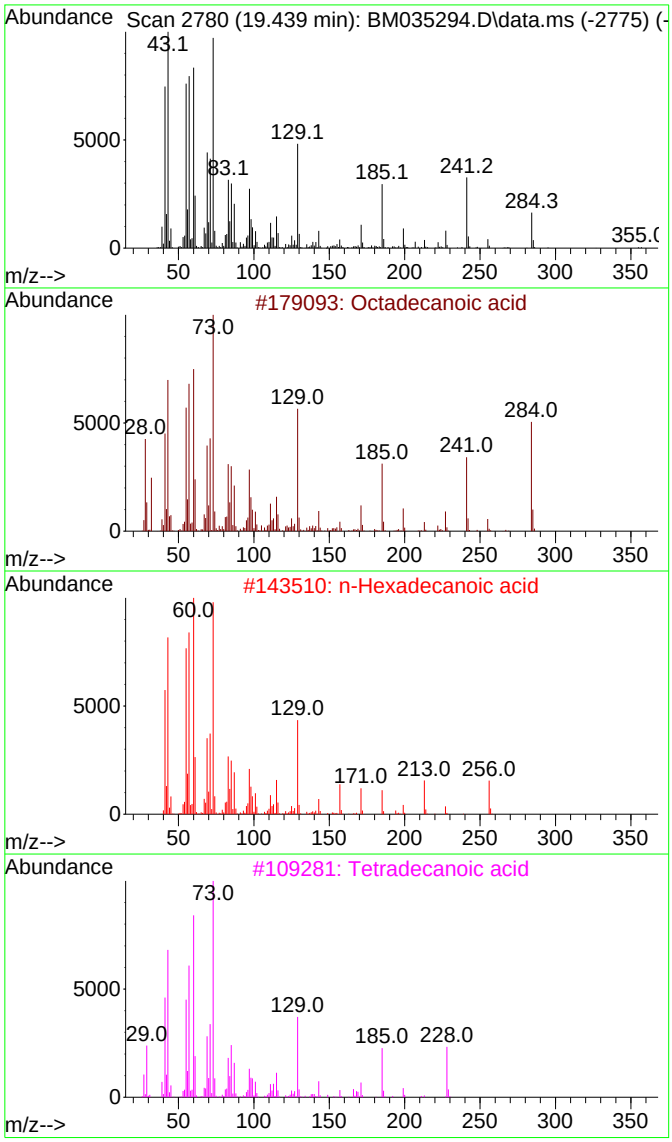
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

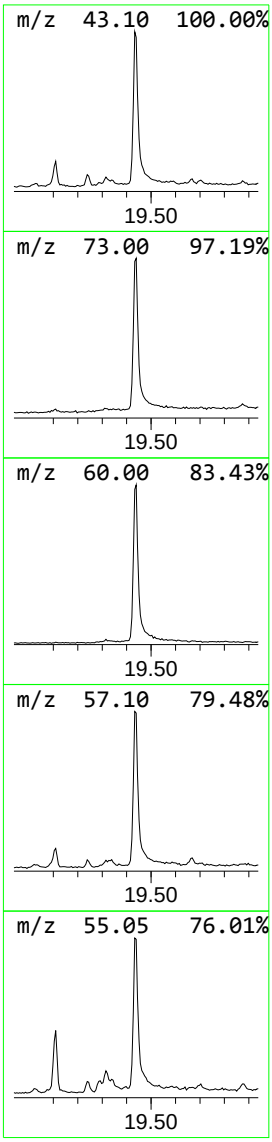
****

Peak Number 6 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.439	10.35 ng	1014530	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052722\
Data File : BM035294.D
Acq On : 27 May 2022 18:11
Operator : CG/JU
Sample : N2930-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P005-SS003-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

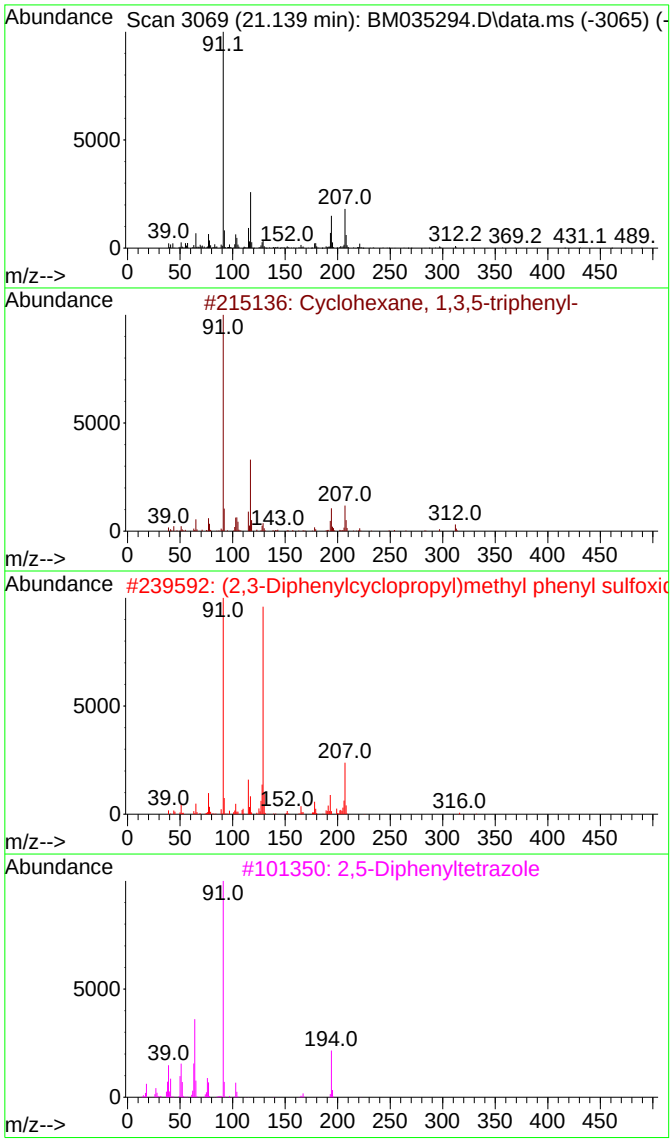
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

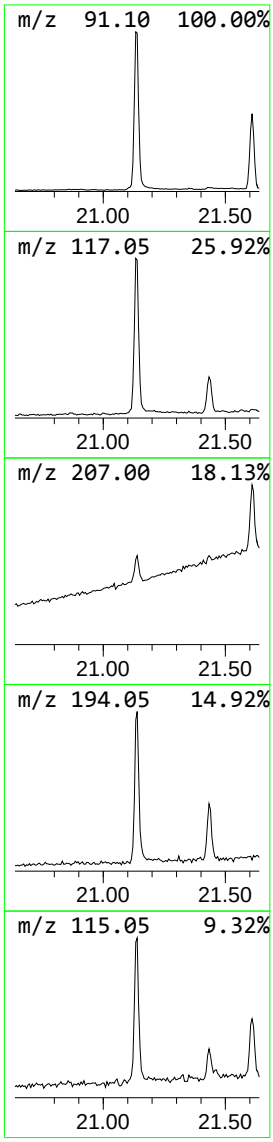
****

Peak Number 7 Cyclohexane, 1,3,5-triphenyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.139	4.71 ng	461790	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,3,5-triphenyl-	312	C24H24	028336-57-4	50
2	(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	47
3	2,5-Diphenyltetrazole	222	C13H10N4	018039-45-7	27
4	Carbonic acid, monoamide, N-benz...	207	C12H17NO2	1000451-48-5	22
5	2-Propenoic acid, 3-[(phenylmeth...	194	C10H10O2S	013831-01-1	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052722\
Data File : BM035294.D
Acq On : 27 May 2022 18:11
Operator : CG/JU
Sample : N2930-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P005-SS003-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

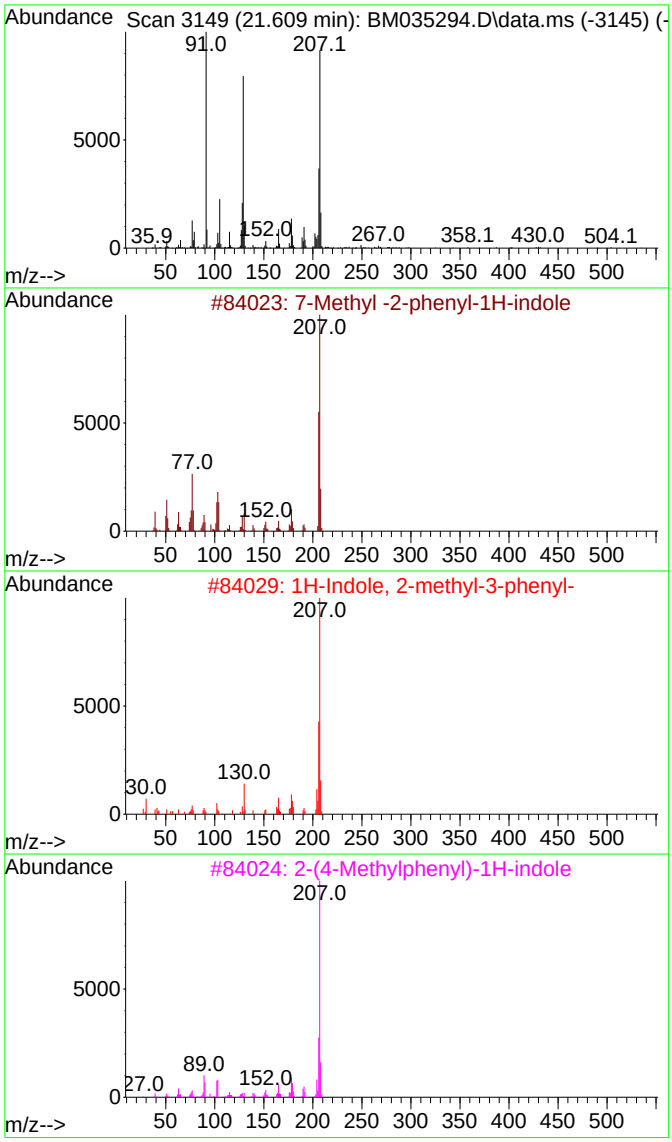
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

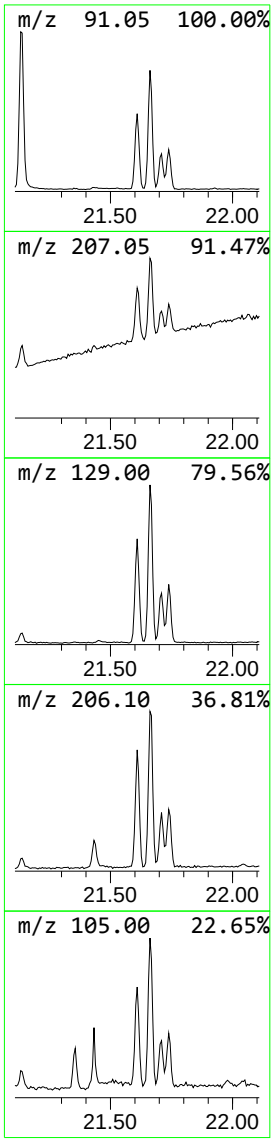
****

Peak Number 8 unknown21.609 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.609	3.87 ng	379399	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Methyl -2-phenyl-1H-indole	207	C15H13N	059541-82-1	46
2	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	45
3	2-(4-Methylphenyl)-1H-indole	207	C15H13N	055577-25-8	45
4	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	43
5	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052722\
Data File : BM035294.D
Acq On : 27 May 2022 18:11
Operator : CG/JU
Sample : N2930-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P005-SS003-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.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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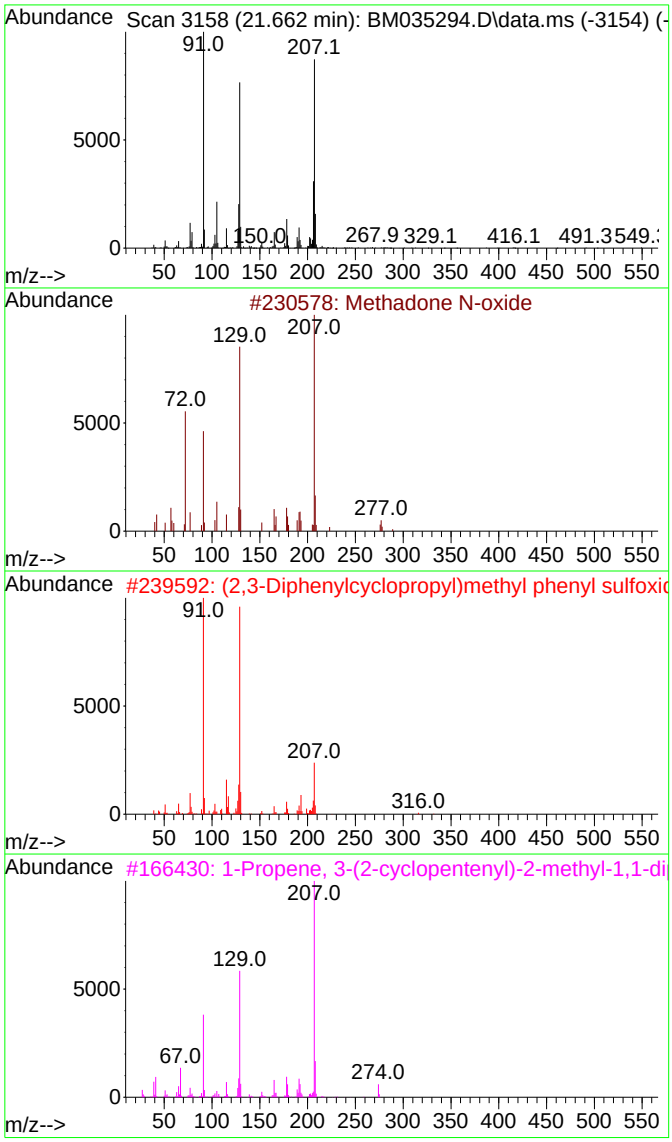
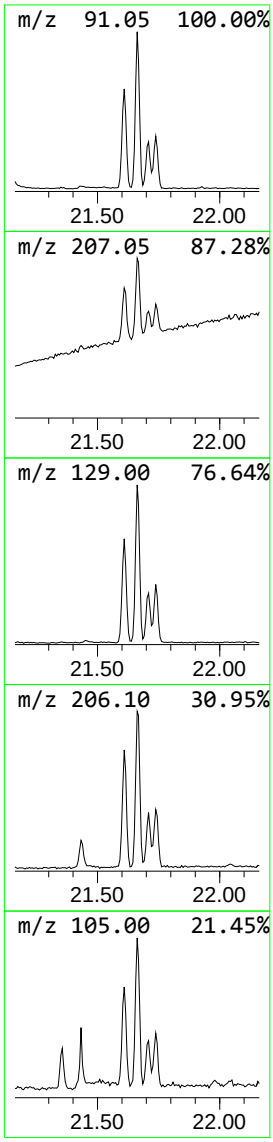
Peak Number 9 Methadone N-oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.662	5.22 ng	511734	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methadone N-oxide	325	C21H27NO2	1000120-80-7	64
2	(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	53
3	1-Propene, 3-(2-cyclopentenyl)-2...	274	C21H22	1010154-23-3	53
4	2-(4-Methylphenyl)-1H-indole	207	C15H13N	055577-25-8	50
5	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052722\
Data File : BM035294.D
Acq On : 27 May 2022 18:11
Operator : CG/JU
Sample : N2930-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P005-SS003-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.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
Ethylbenzene	5.387	3.4	ng	130557	1	7.875	767405	20.0
Bicyclo[4.2.0]o...	5.863	2.5	ng	97903	1	7.875	767405	20.0
Cyclohexane, 1-...	13.398	2.6	ng	163512	3	14.510	1232840	20.0
n-Hexadecanoic ...	18.162	14.3	ng	976674	4	17.256	1364990	20.0
11-Octadecenoic...	19.109	3.2	ng	217256	4	17.256	1364990	20.0
Octadecanoic acid	19.439	10.4	ng	1014530	5	21.433	1961010	20.0
Cyclohexane, 1,...	21.139	4.7	ng	461790	5	21.433	1961010	20.0
unknown21.609	21.609	3.9	ng	379399	5	21.433	1961010	20.0
Methadone N-oxide	21.662	5.2	ng	511734	5	21.433	1961010	20.0