LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091824\
Data File : BM047563.D
Acq On : 18 Sep 2024 19:45
Operator : RC/JU
Sample : P4087-13
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-614-COMP-03

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-BM091424.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047563.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.040	157	162	168	rBV	86331	116282	1.52%	0.254%
2	4.963	314	319	327	rVB	197101	282321	3.68%	0.616%
3	5.422	390	397	405	rBV	3287538	4642277	60.57%	10.134%
4	5.498	405	410	420	rVB	90789	199679	2.61%	0.436%
5	7.010	660	667	676	rBV	3407490	5174374	67.51%	11.296%
6	7.851	803	810	817	rVB	870596	1357170	17.71%	2.963%
7	9.004	995	1006	1014	rBV	1896464	3074017	40.11%	6.710%
8	9.569	1097	1102	1110	rVB	53655	87330	1.14%	0.191%
9	10.645	1278	1285	1292	rBV	1090868	1813128	23.66%	3.958%
10	13.104	1696	1703	1715	rBV	4285484	6083977	79.38%	13.281%
11	14.480	1930	1937	1943	rBV	1442821	2065640	26.95%	4.509%
12	15.833	2162	2167	2175	rBV	183238	252934	3.30%	0.552%
13	15.962	2181	2189	2207	rBV	2808896	3876840	50.58%	8.463%
14	17.215	2395	2402	2407	rBV	1573005	2199279	28.70%	4.801%
15	17.256	2407	2409	2416	rVV	87042	113014	1.47%	0.247%
16	18.109	2547	2554	2564	rBV2	326611	572959	7.48%	1.251%
17	19.262	2745	2750	2759	rBV	306896	434863	5.67%	0.949%
18	19.386	2767	2771	2774	rBV2	83837	103911	1.36%	0.227%
19	19.627	2808	2812	2819	rVB	256992	368731	4.81%	0.805%
20	19.833	2841	2847	2857	rBV	6341379	7664272	100.00%	16.731%
21	21.121	3062	3066	3073	rBV2	260050	397502	5.19%	0.868%
22	21.439	3114	3120	3126	rBV2	1605933	2587639	33.76%	5.649%
23	24.474	3628	3636	3645	rBV	966296	2340926	30.54%	5.110%

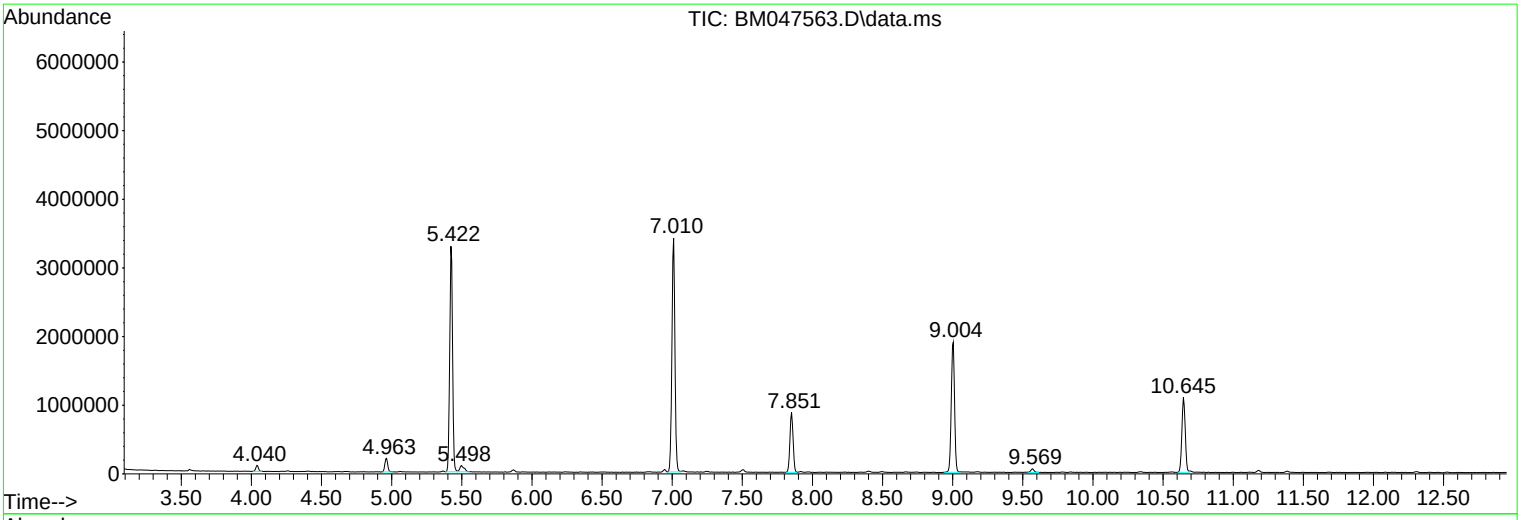
Sum of corrected areas: 45809065

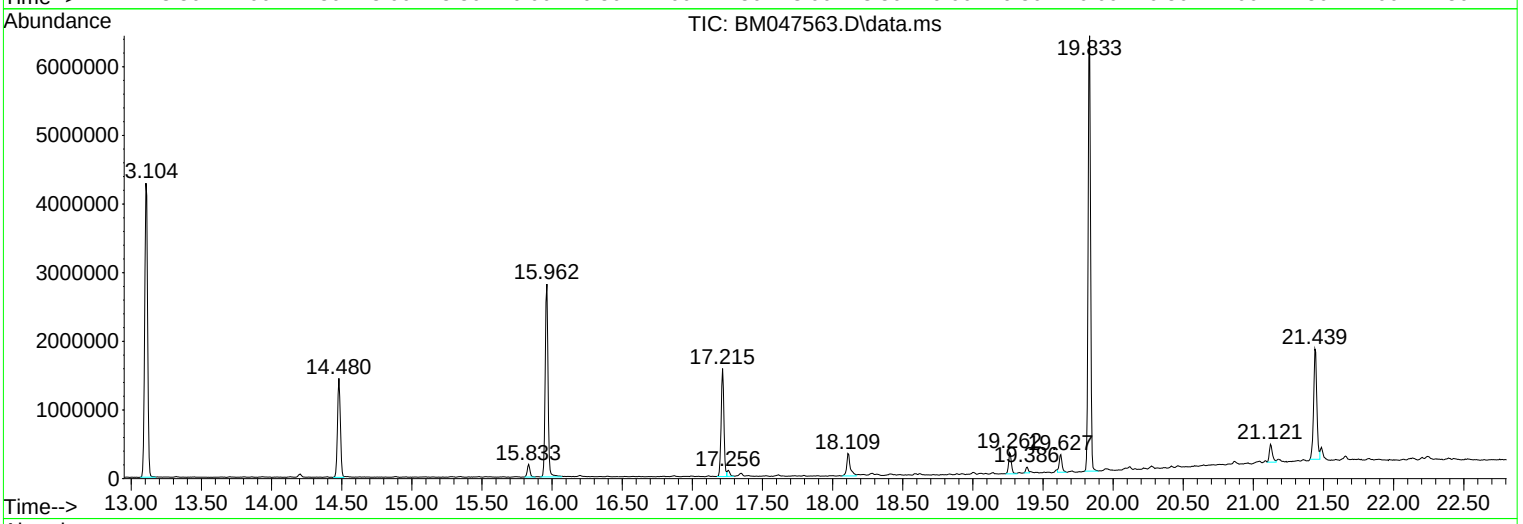
Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091824\
Data File : BM047563.D
Acq On : 18 Sep 2024 19:45
Operator : RC/JU
Sample : P4087-13
Misc :
ALS Vial : 12 Sample Multiplier: 1

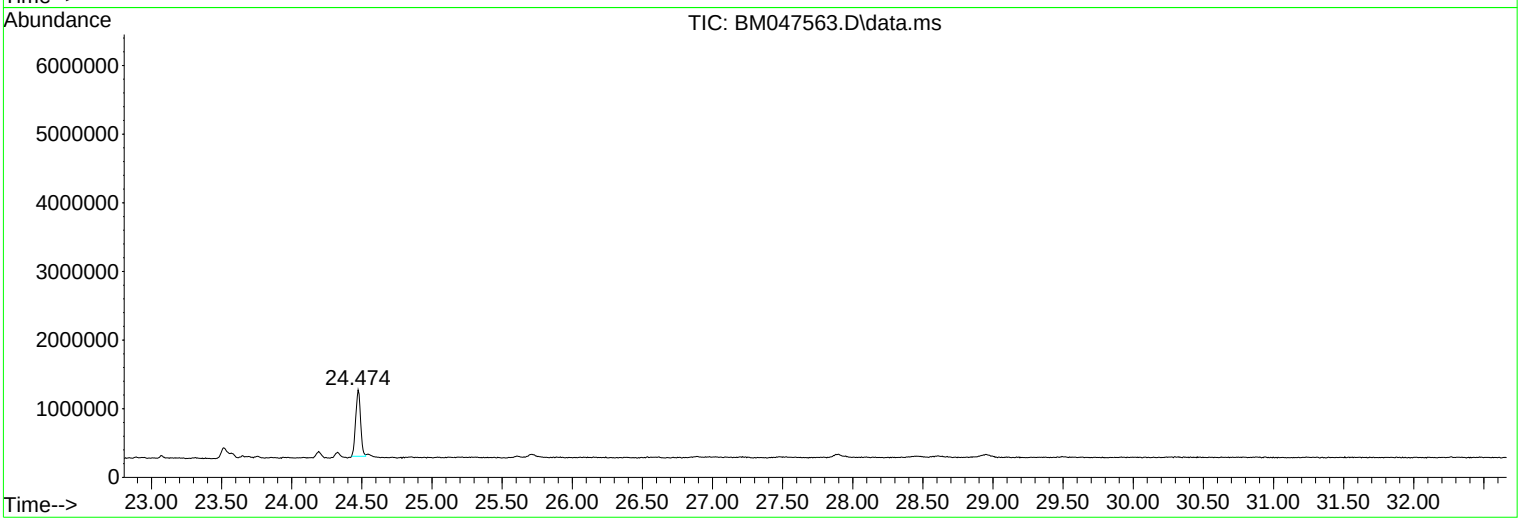
Instrument :
BNA_M
ClientSampleId :
NB-614-COMP-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.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\BM091824\
Data File : BM047563.D
Acq On : 18 Sep 2024 19:45
Operator : RC/JU
Sample : P4087-13
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-614-COMP-03

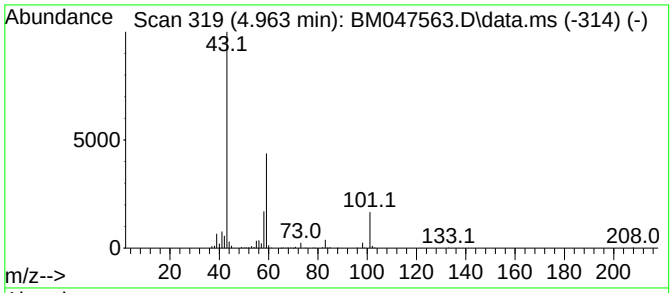
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

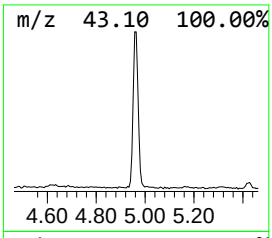
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

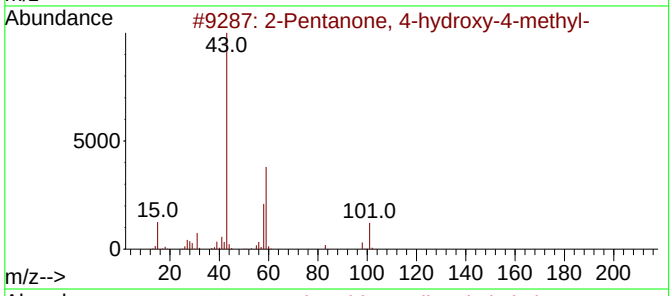
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

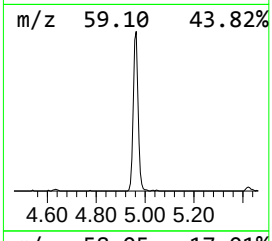
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.963	4.16 ng	282321	1,4-Dichlorobenzene-d4	7.851

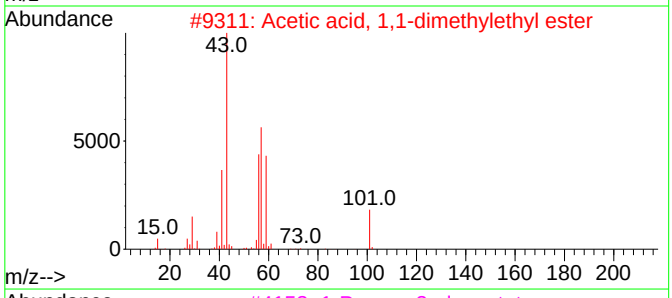
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	78
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	45
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9

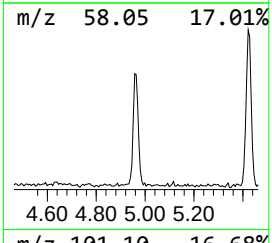


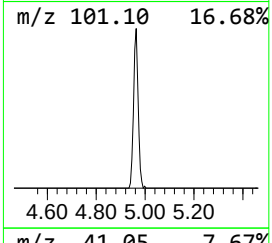


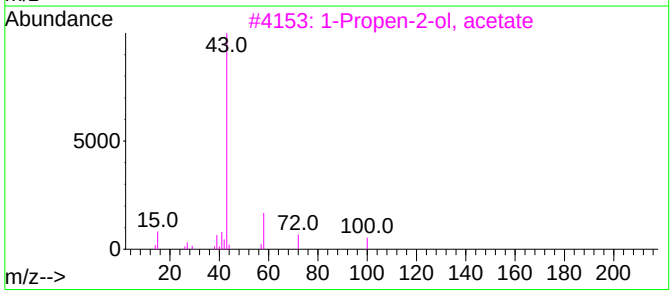


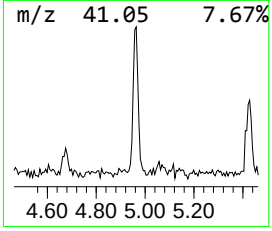












Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091824\
Data File : BM047563.D
Acq On : 18 Sep 2024 19:45
Operator : RC/JU
Sample : P4087-13
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-614-COMP-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

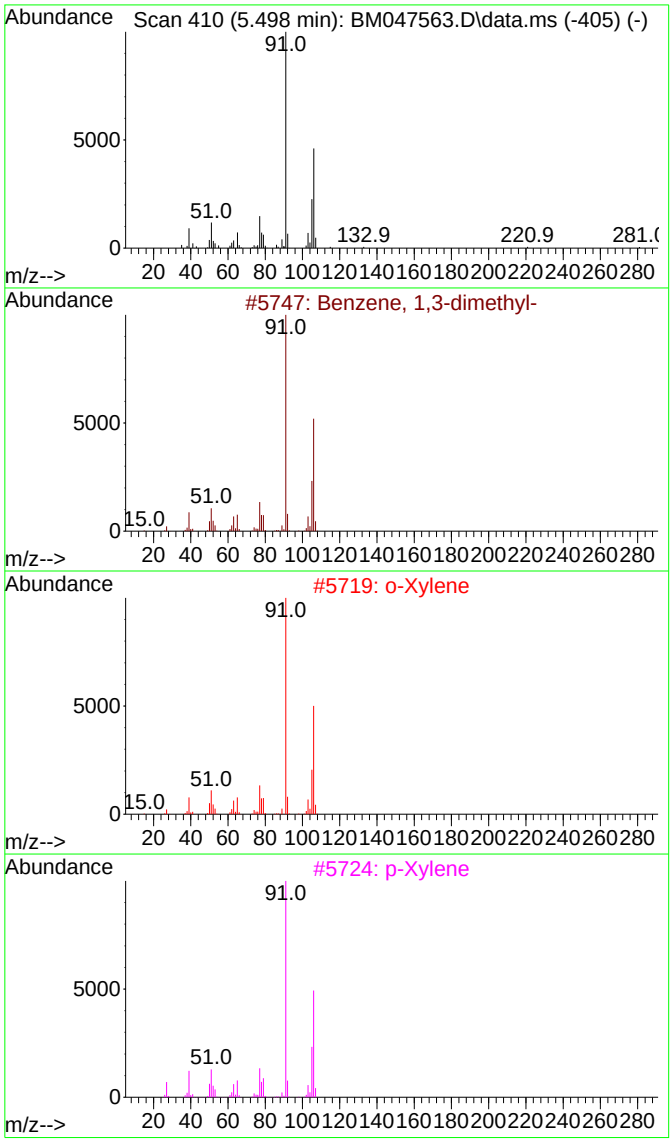
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

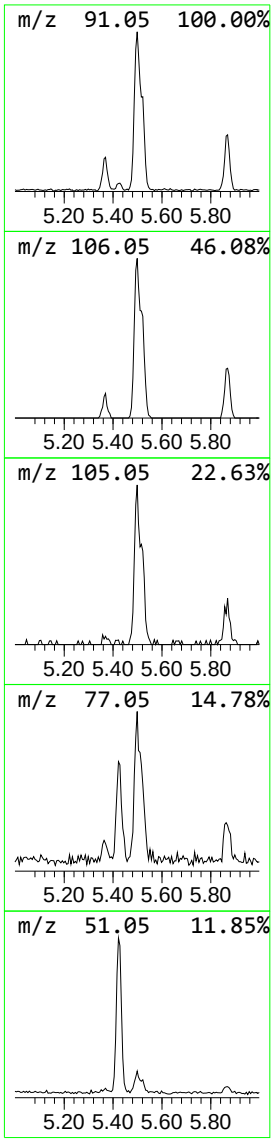
****

Peak Number 2 Benzene, 1,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.498	2.94 ng	199679	1,4-Dichlorobenzene-d4	7.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	97
2	o-Xylene	106	C8H10	000095-47-6	97
3	p-Xylene	106	C8H10	000106-42-3	95
4	1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	91
5	Ethylbenzene	106	C8H10	000100-41-4	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091824\
Data File : BM047563.D
Acq On : 18 Sep 2024 19:45
Operator : RC/JU
Sample : P4087-13
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-614-COMP-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

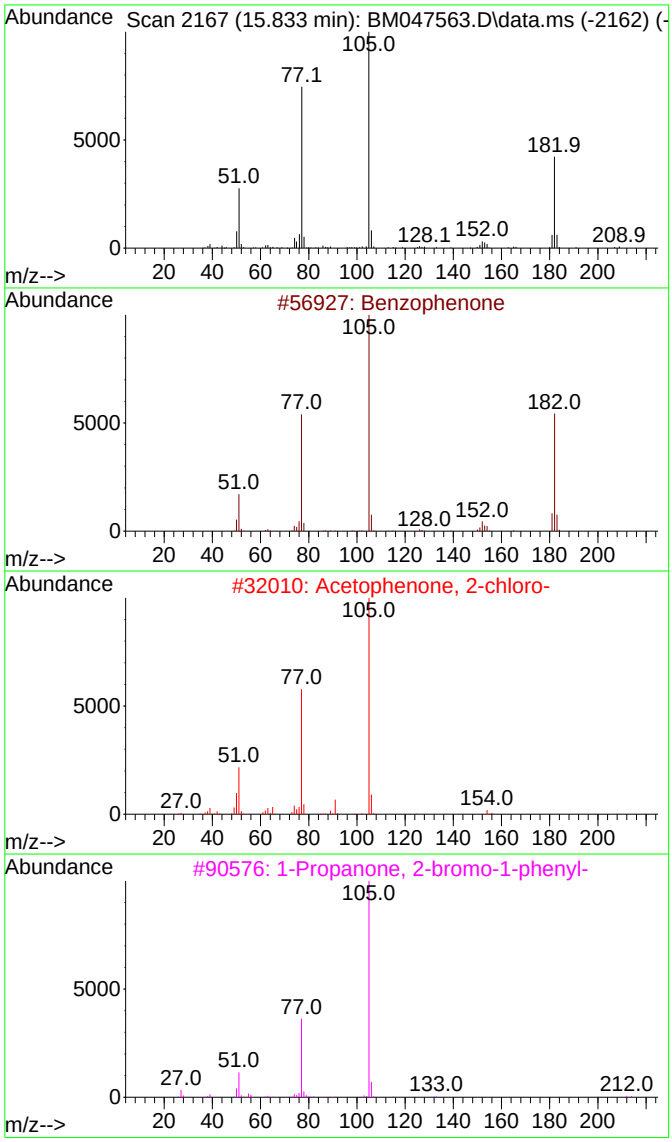
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

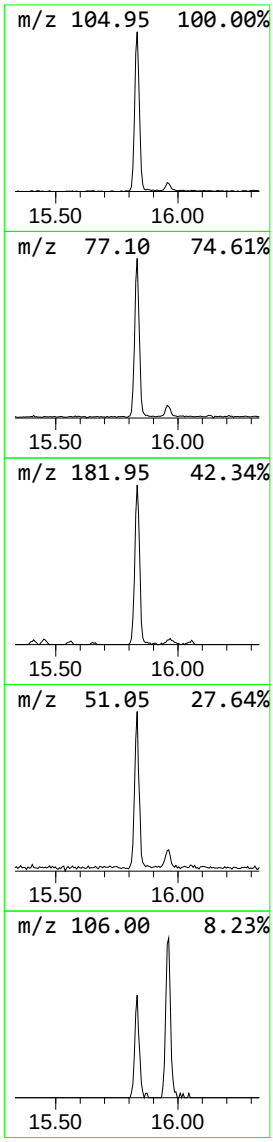
****

Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.833	2.45 ng	252934	Acenaphthene-d10	14.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	95
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	58
3	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	53
4	acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	53
5	2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091824\
Data File : BM047563.D
Acq On : 18 Sep 2024 19:45
Operator : RC/JU
Sample : P4087-13
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-614-COMP-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

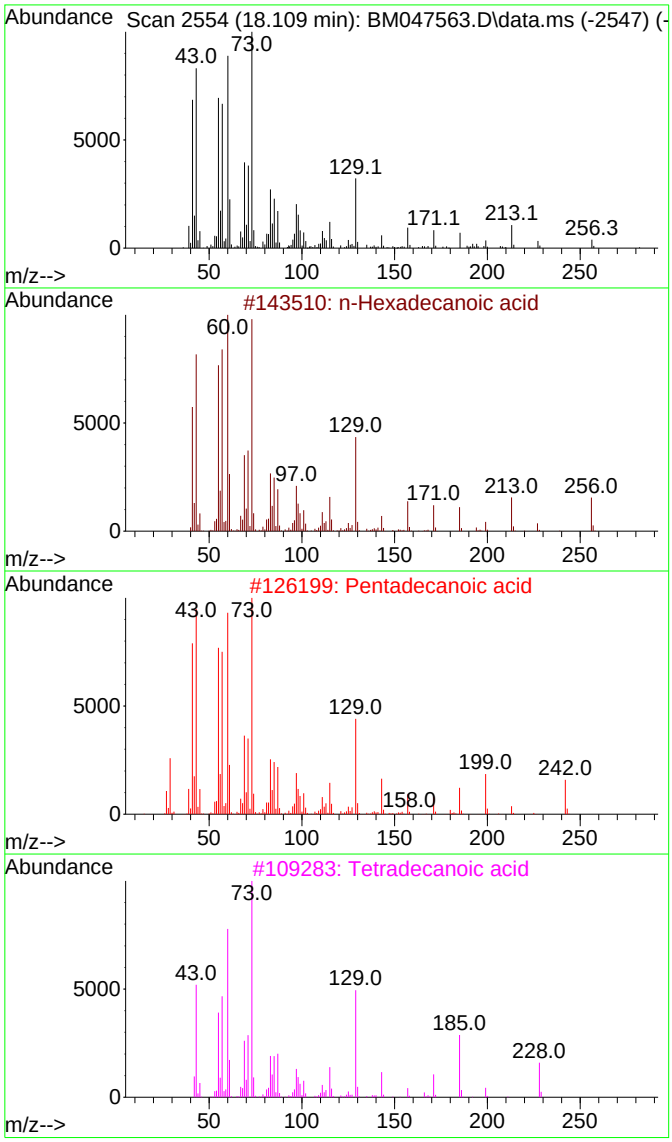
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

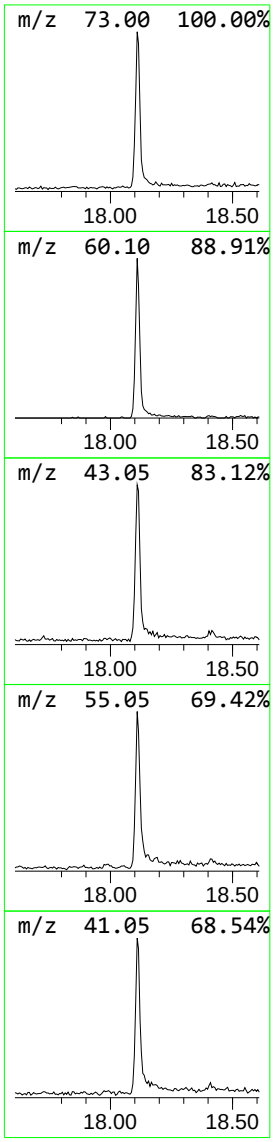
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.109	5.21 ng	572959	Phenanthrene-d10	17.215

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	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091824\
Data File : BM047563.D
Acq On : 18 Sep 2024 19:45
Operator : RC/JU
Sample : P4087-13
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-614-COMP-03

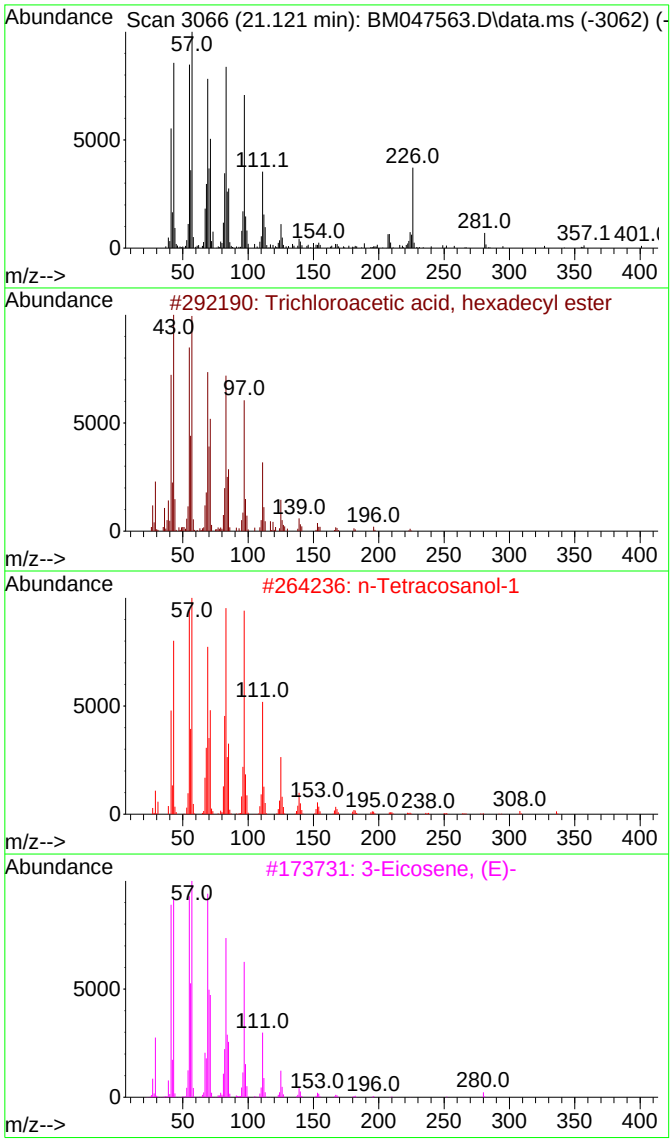
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

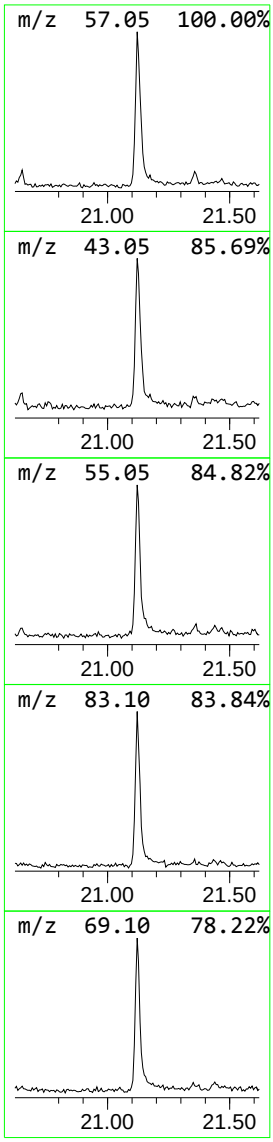
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Trichloroacetic acid, hexad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.121	3.07 ng	397502	Chrysene-d12	21.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	90
4	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	90
5	1-Hexacosanol	382	C26H54O	000506-52-5	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091824\
Data File : BM047563.D
Acq On : 18 Sep 2024 19:45
Operator : RC/JU
Sample : P4087-13
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
NB-614-COMP-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.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-...	4.963	4.2	ng	282321	1	7.851	1357170	20.0
Benzene, 1,3-di...	5.498	2.9	ng	199679	1	7.851	1357170	20.0
Benzophenone	15.833	2.5	ng	252934	3	14.480	2065640	20.0
n-Hexadecanoic ...	18.109	5.2	ng	572959	4	17.215	2199280	20.0
Trichloroacetic...	21.121	3.1	ng	397502	5	21.439	2587640	20.0