LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082724\
Data File : BM047364.D
Acq On : 27 Aug 2024 15:17
Operator : RC/JU
Sample : P3741-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TR-05-08262024

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-BM082624.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047364.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.257	60	63	79	rBV	164229	270838	2.84%	0.409%
2	4.563	276	285	293	rBV	171453	259460	2.72%	0.392%
3	5.010	355	361	377	rBV	2837996	4475656	46.93%	6.763%
4	6.575	620	627	640	rBV	2892462	4722590	49.52%	7.136%
5	6.981	692	696	708	rBV	102717	198424	2.08%	0.300%
6	7.351	751	759	769	rBV	1085698	1694573	17.77%	2.561%
7	8.498	947	954	976	rBV	1894903	3174741	33.29%	4.797%
8	10.104	1218	1227	1243	rBV	1395883	2362719	24.77%	3.570%
9	10.869	1349	1357	1368	rBV	204627	425058	4.46%	0.642%
10	12.616	1647	1654	1670	rVB	5125788	7649740	80.21%	11.559%
11	13.733	1839	1844	1850	rVB	86509	144226	1.51%	0.218%
12	14.010	1885	1891	1899	rBV	2192143	3267064	34.25%	4.937%
13	14.245	1925	1931	1933	rBV	1110509	1577098	16.54%	2.383%
14	14.268	1933	1935	1946	rVB	1276939	1445724	15.16%	2.185%
15	14.904	2039	2043	2049	rVB2	106225	128597	1.35%	0.194%
16	15.527	2142	2149	2158	rBV	4361582	6116854	64.13%	9.243%
17	15.774	2186	2191	2194	rBV2	164612	248452	2.60%	0.375%
18	16.568	2322	2326	2330	rBV	163022	208041	2.18%	0.314%
19	16.780	2356	2362	2366	rBV	2764865	3827422	40.13%	5.783%
20	16.821	2366	2369	2377	rVV	390231	562032	5.89%	0.849%
21	16.915	2380	2385	2392	rVB	155347	251848	2.64%	0.381%
22	17.309	2448	2452	2456	rBV	173673	206702	2.17%	0.312%
23	17.486	2478	2482	2491	rVB3	142674	202320	2.12%	0.306%
24	17.656	2508	2511	2516	rBV	141936	193070	2.02%	0.292%
25	17.715	2516	2521	2530	rBV2	1150944	1674802	17.56%	2.531%
26	17.851	2540	2544	2548	rBV2	141952	221432	2.32%	0.335%
27	18.003	2567	2570	2575	rVB	147492	178614	1.87%	0.270%
28	18.592	2667	2670	2674	rBV	128216	185266	1.94%	0.280%
29	18.645	2675	2679	2682	rVV4	461578	733288	7.69%	1.108%
30	18.674	2682	2684	2691	rVB3	447996	524674	5.50%	0.793%
31	18.815	2705	2708	2711	rBV	107051	128310	1.35%	0.194%
32	18.862	2711	2716	2720	rBV	899976	1300473	13.64%	1.965%
33	19.015	2739	2742	2748	rBV	413596	566927	5.94%	0.857%
34	19.227	2774	2778	2786	rVB	757993	1155828	12.12%	1.746%
35	19.450	2810	2816	2821	rVB	7801904	9537564	100.00%	14.411%
36	20.756	3035	3038	3041	rVB2	528645	575699	6.04%	0.870%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082724\
Data File : BM047364.D
Acq On : 27 Aug 2024 15:17
Operator : RC/JU
Sample : P3741-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TR-05-08262024

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-BM082624.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.027	3079	3084	3088	rVB	2089144	2860963	30.00%	4.323%
38	23.727	3537	3543	3554	rVB	1339553	2923789	30.66%	4.418%

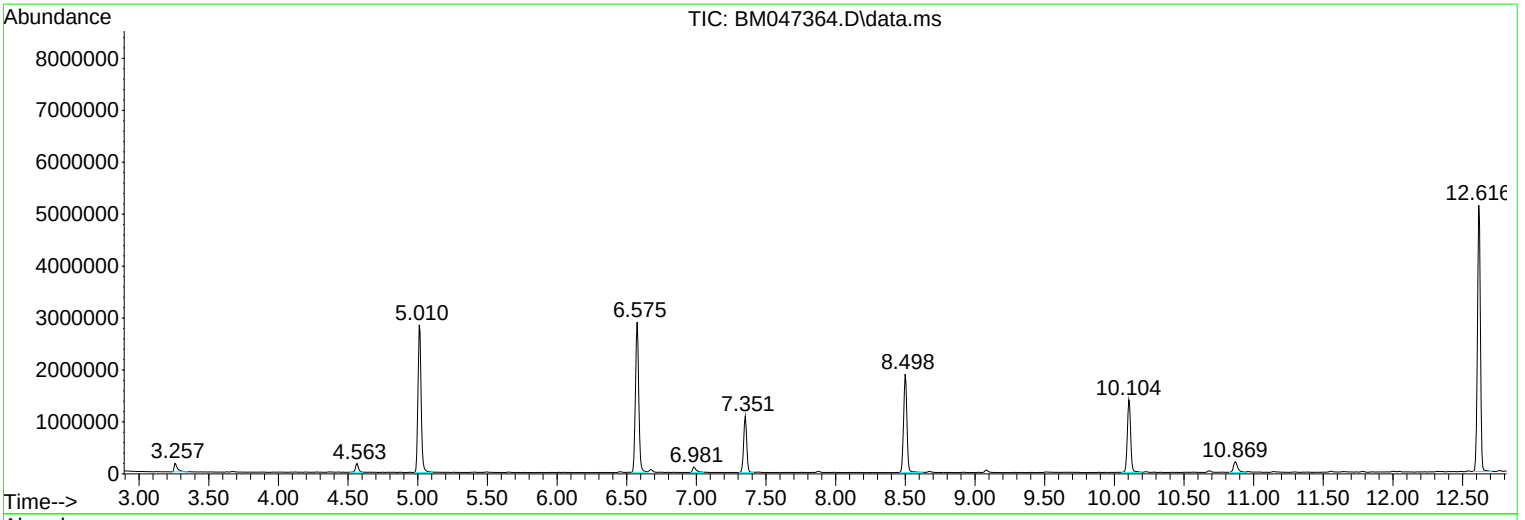
Sum of corrected areas: 66180878

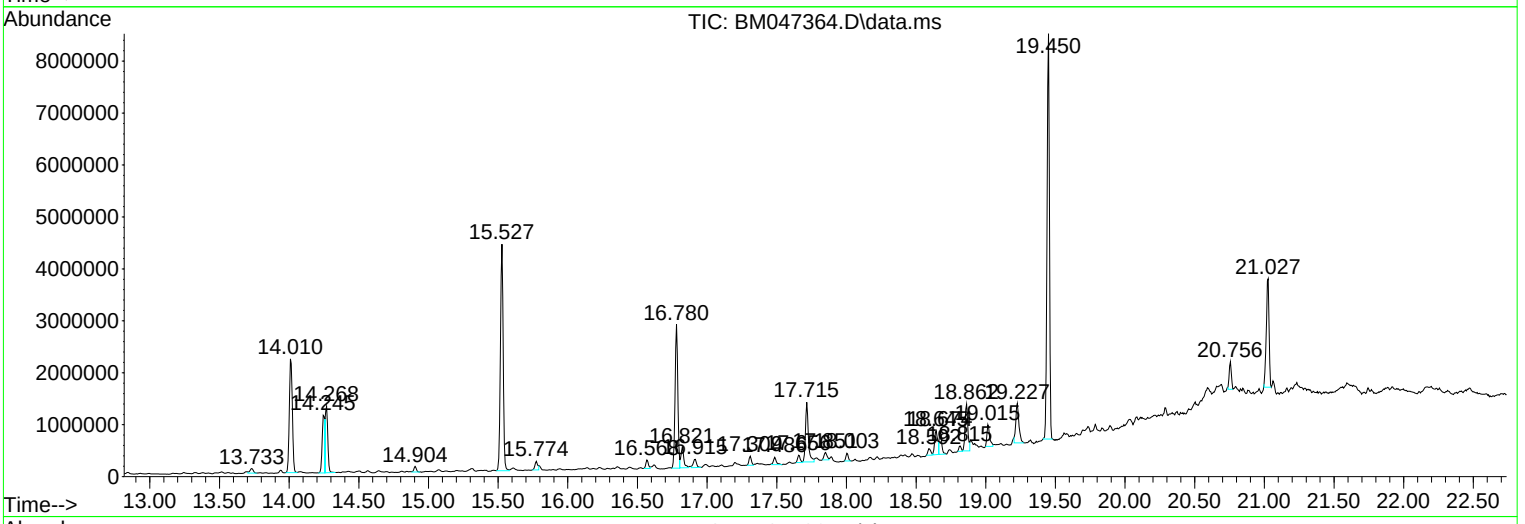
Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082724\
Data File : BM047364.D
Acq On : 27 Aug 2024 15:17
Operator : RC/JU
Sample : P3741-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

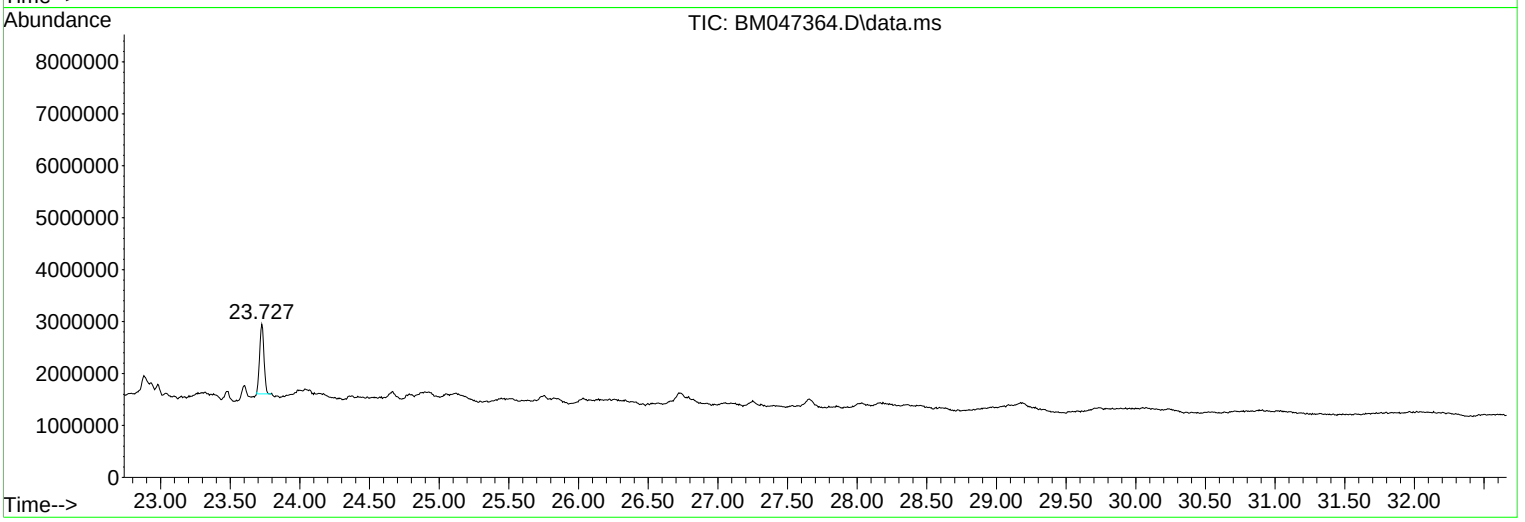
Instrument :
BNA_M
ClientSampleId :
TR-05-08262024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.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\BM082724\
Data File : BM047364.D
Acq On : 27 Aug 2024 15:17
Operator : RC/JU
Sample : P3741-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TR-05-08262024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

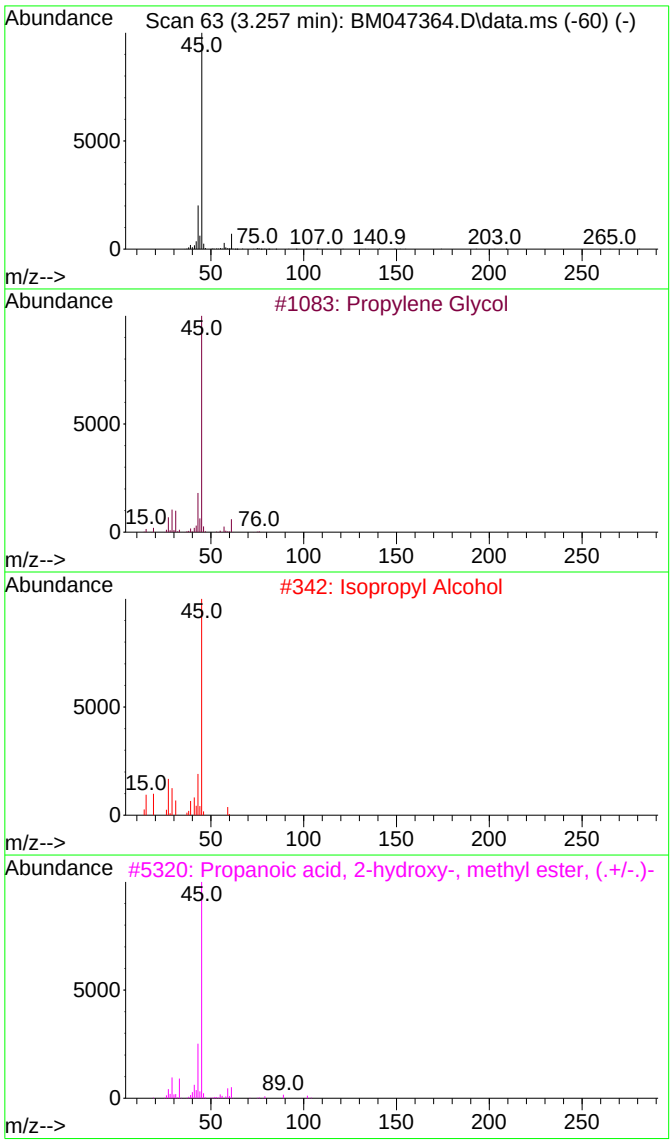
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

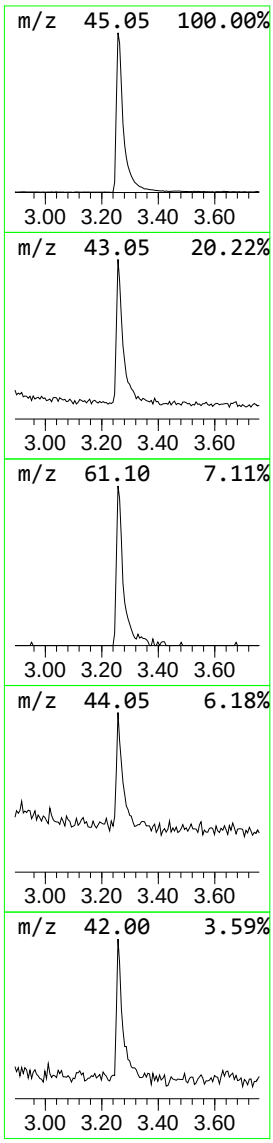
****

Peak Number 1 Propylene Glycol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.257	3.20 ng	270838	1,4-Dichlorobenzene-d4	7.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	90
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
3	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
4	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
5	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082724\
Data File : BM047364.D
Acq On : 27 Aug 2024 15:17
Operator : RC/JU
Sample : P3741-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TR-05-08262024

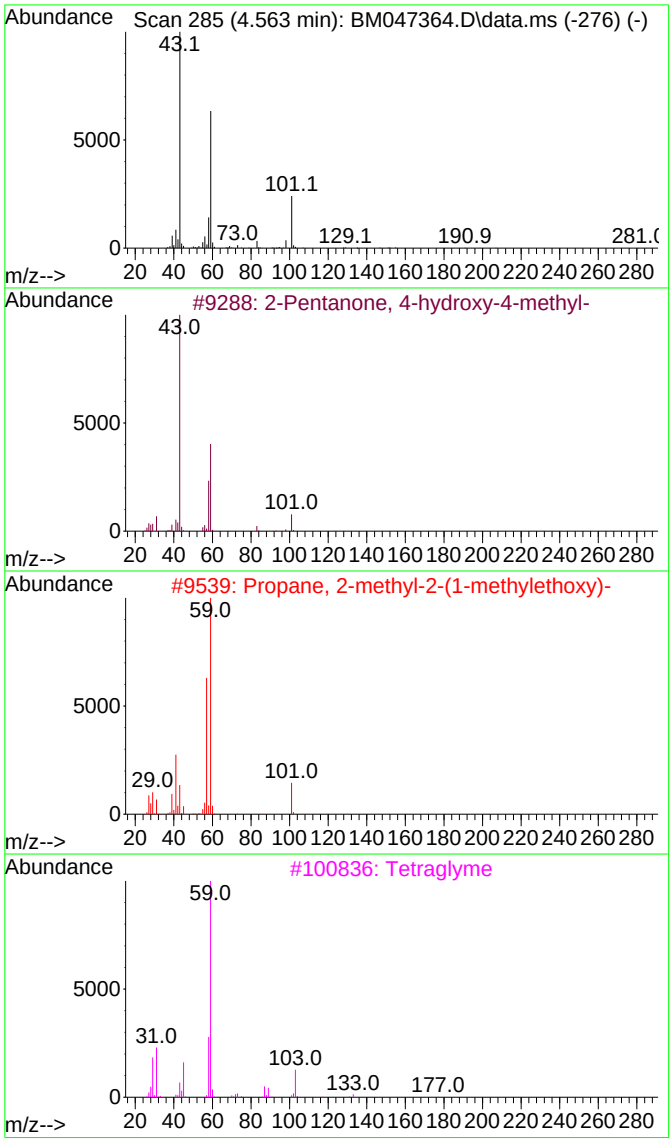
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

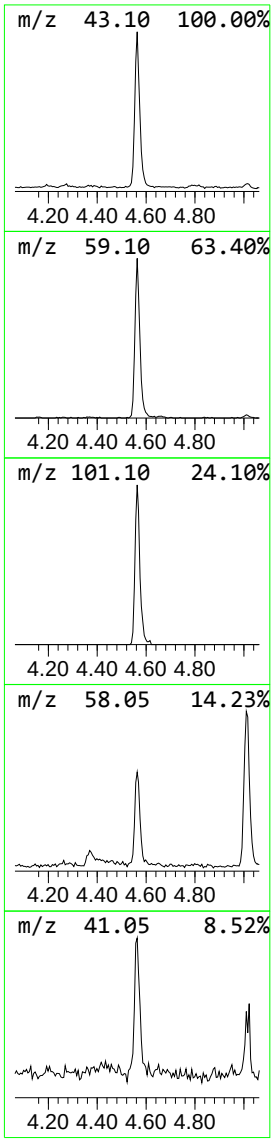
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.563	3.06 ng	259460	1,4-Dichlorobenzene-d4	7.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	Tetraglyme	222	C10H22O5	000143-24-8	25
4	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
5	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082724\
Data File : BM047364.D
Acq On : 27 Aug 2024 15:17
Operator : RC/JU
Sample : P3741-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TR-05-08262024

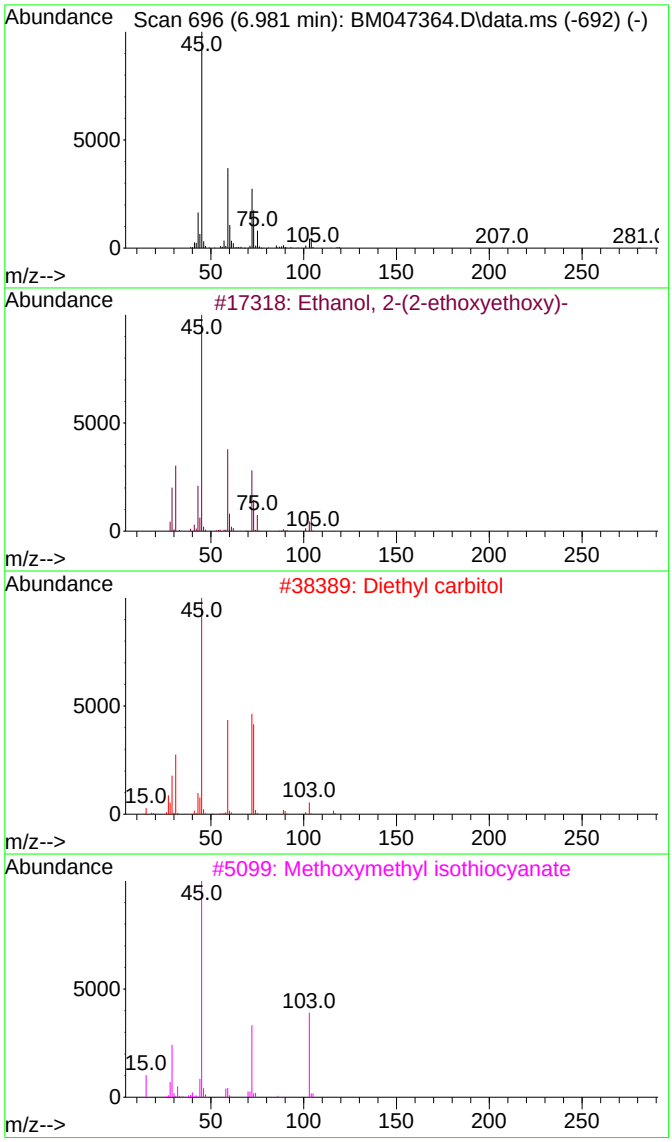
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

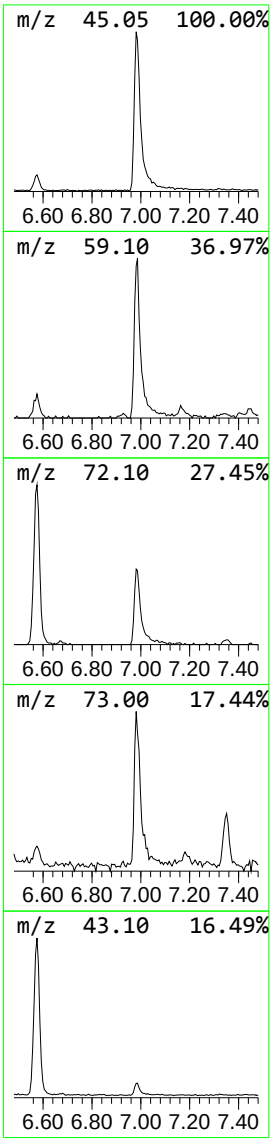
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.981	2.34 ng	198424	1,4-Dichlorobenzene-d4	7.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2	Diethyl carbitol	162	C8H18O3	000112-36-7	72
3	Methoxymethyl isothiocyanate	103	C3H5NOS	019900-84-6	53
4	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
5	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082724\
Data File : BM047364.D
Acq On : 27 Aug 2024 15:17
Operator : RC/JU
Sample : P3741-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TR-05-08262024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

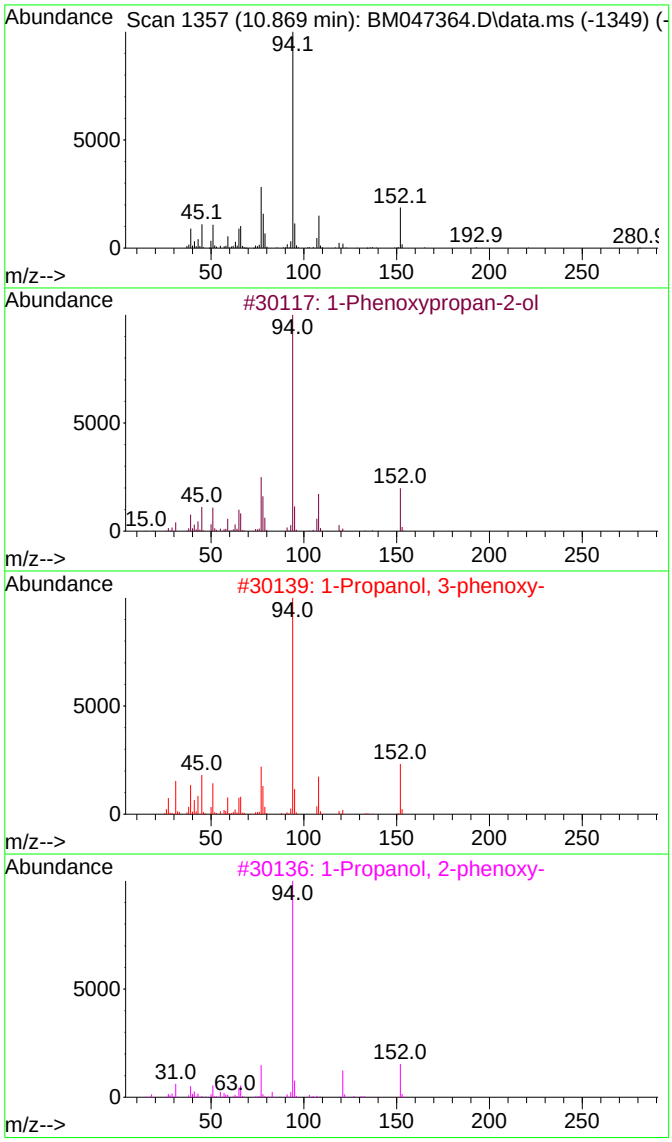
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

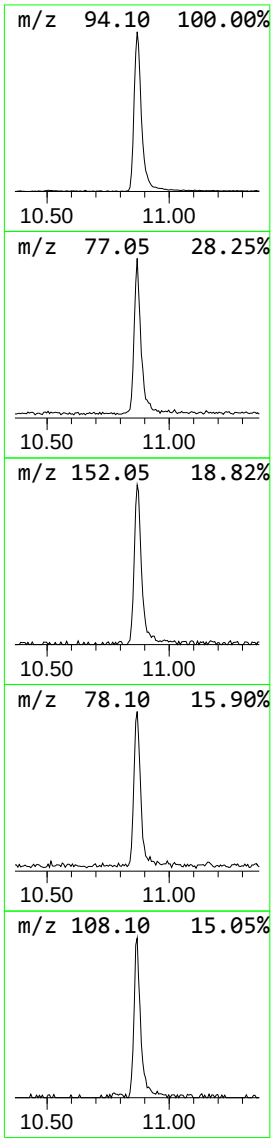
****

Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.869	3.60 ng	425058	Naphthalene-d8	10.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	70
3	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
5	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082724\
Data File : BM047364.D
Acq On : 27 Aug 2024 15:17
Operator : RC/JU
Sample : P3741-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TR-05-08262024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

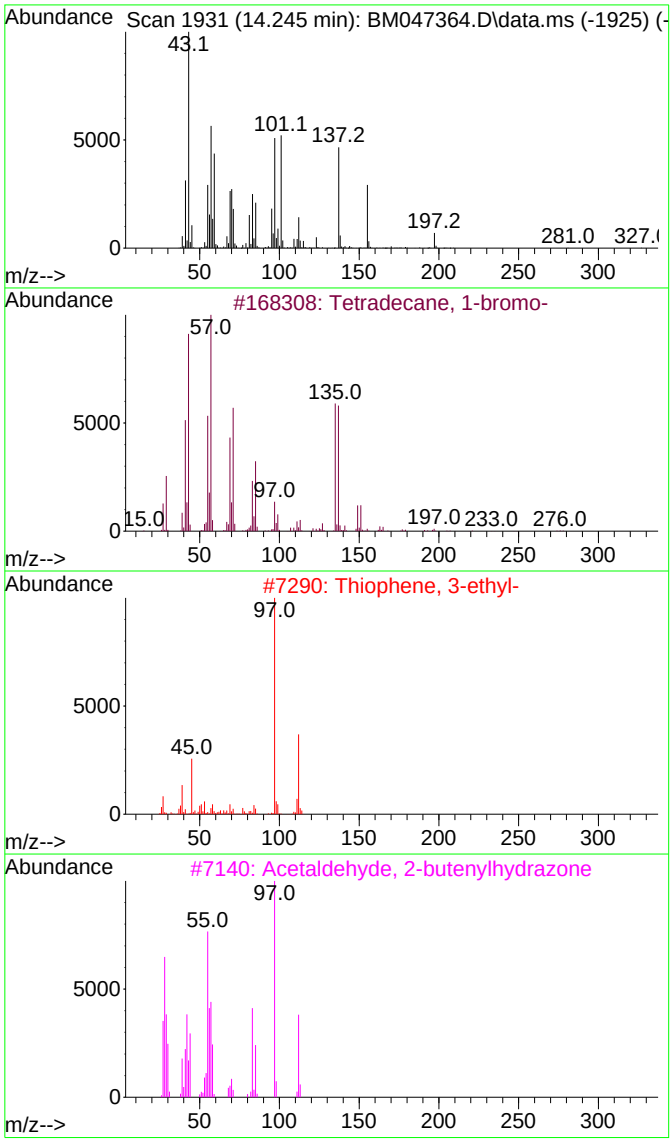
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

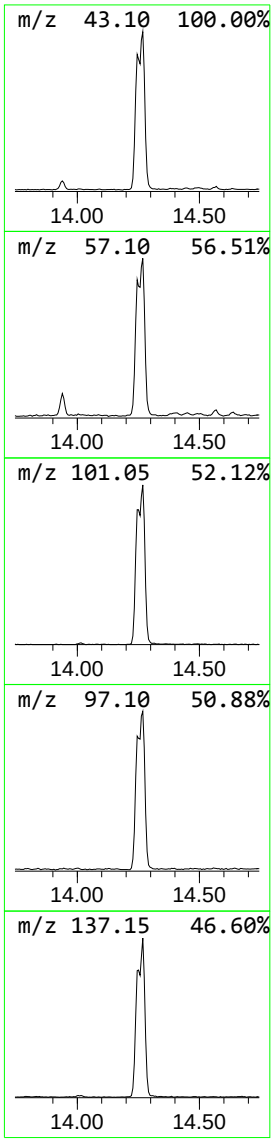
****

Peak Number 5 unknown14.245 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.245	9.65 ng	1577100	Acenaphthene-d10	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane, 1-bromo-	276	C14H29Br	000112-71-0	14
2	Thiophene, 3-ethyl-	112	C6H8S	001795-01-3	11
3	Acetaldehyde, 2-butenylhydrazone	112	C6H12N2	075268-07-4	11
4	Thiophene, 2-ethyl-	112	C6H8S	000872-55-9	11
5	Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	11





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082724\
Data File : BM047364.D
Acq On : 27 Aug 2024 15:17
Operator : RC/JU
Sample : P3741-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TR-05-08262024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

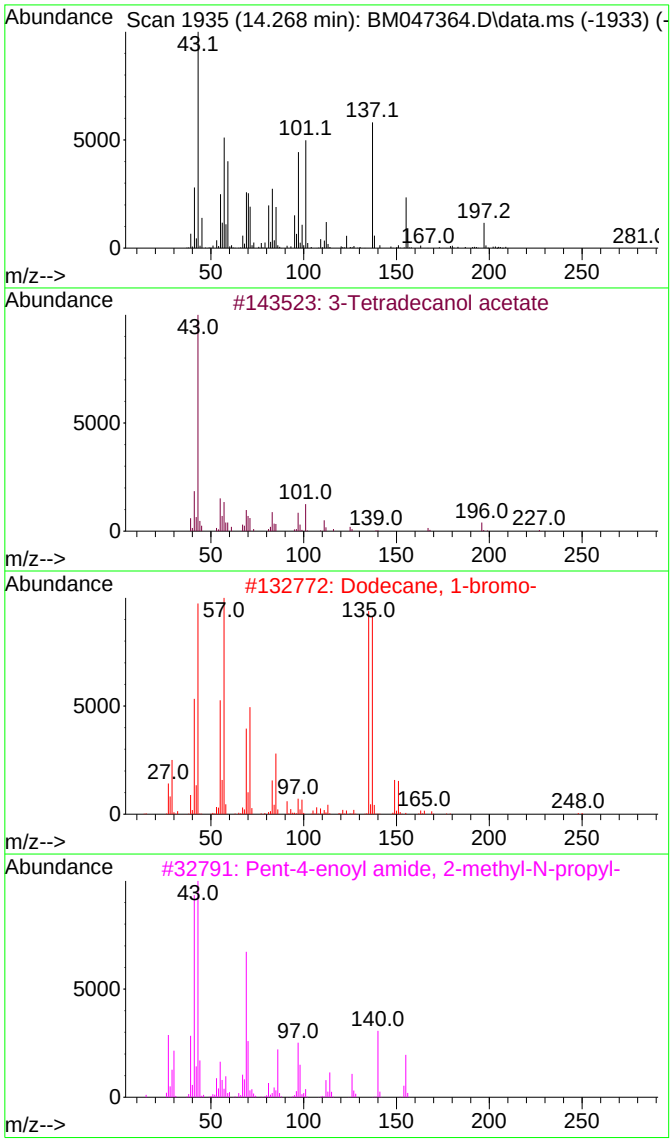
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

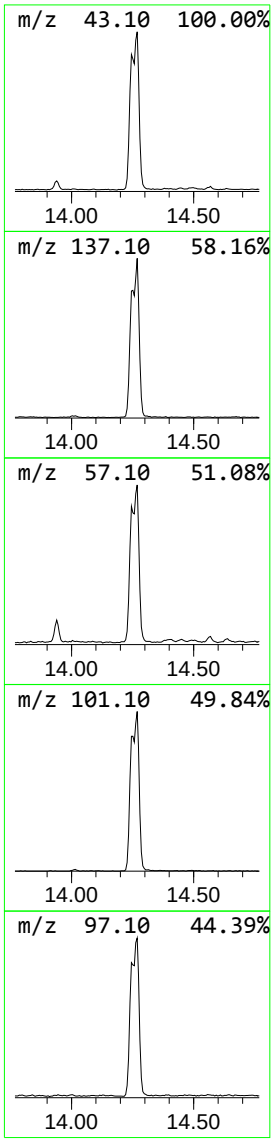
****

Peak Number 6 unknown14.268 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.268	8.85 ng	1445720	Acenaphthene-d10	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Tetradecanol acetate	256	C16H32O2	051354-23-5	12
2	Dodecane, 1-bromo-	248	C12H25Br	000143-15-7	10
3	Pent-4-enoyl amide, 2-methyl-N-p...	155	C9H17NO	1000420-35-2	10
4	Tetradecane, 1-bromo-	276	C14H29Br	000112-71-0	10
5	Butanoic acid, 3-oxo-, 1,1-dimet...	158	C8H14O3	001694-31-1	10





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Data File : BM047364.D
Acq On : 27 Aug 2024 15:17
Operator : RC/JU
Sample : P3741-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TR-05-08262024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

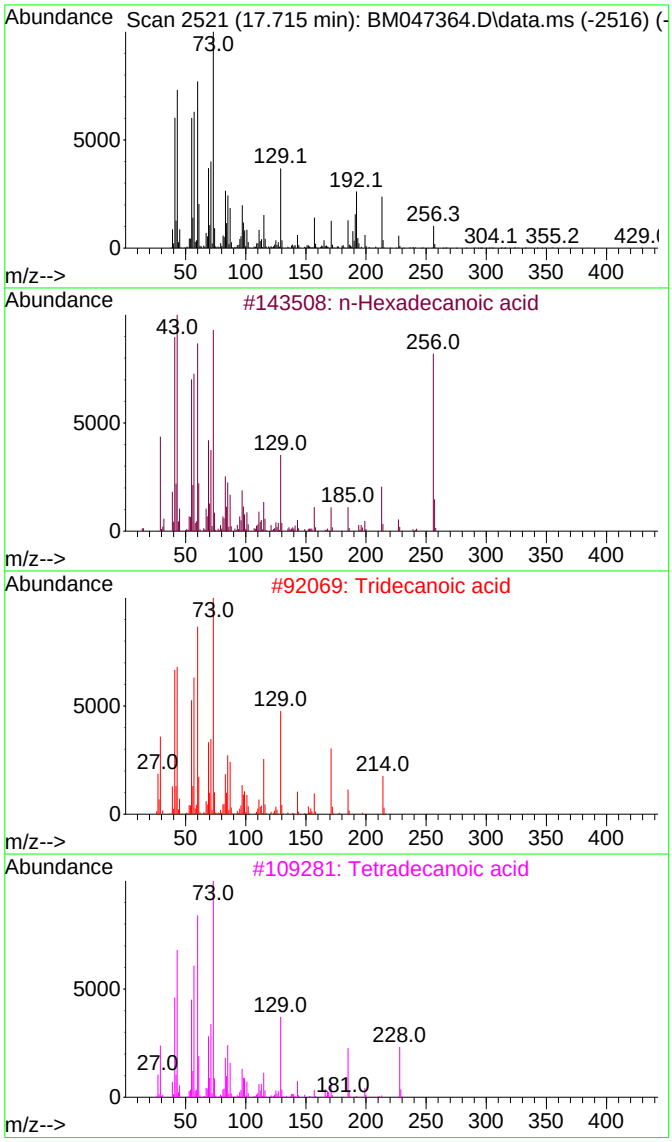
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

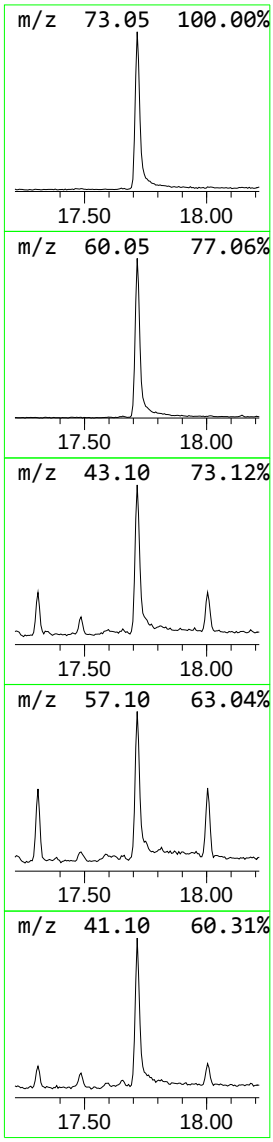
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.715	8.75 ng	1674800	Phenanthrene-d10	16.780

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	92
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	Octadecanoic acid	284	C18H36O2	000057-11-4	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082724\
Data File : BM047364.D
Acq On : 27 Aug 2024 15:17
Operator : RC/JU
Sample : P3741-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TR-05-08262024

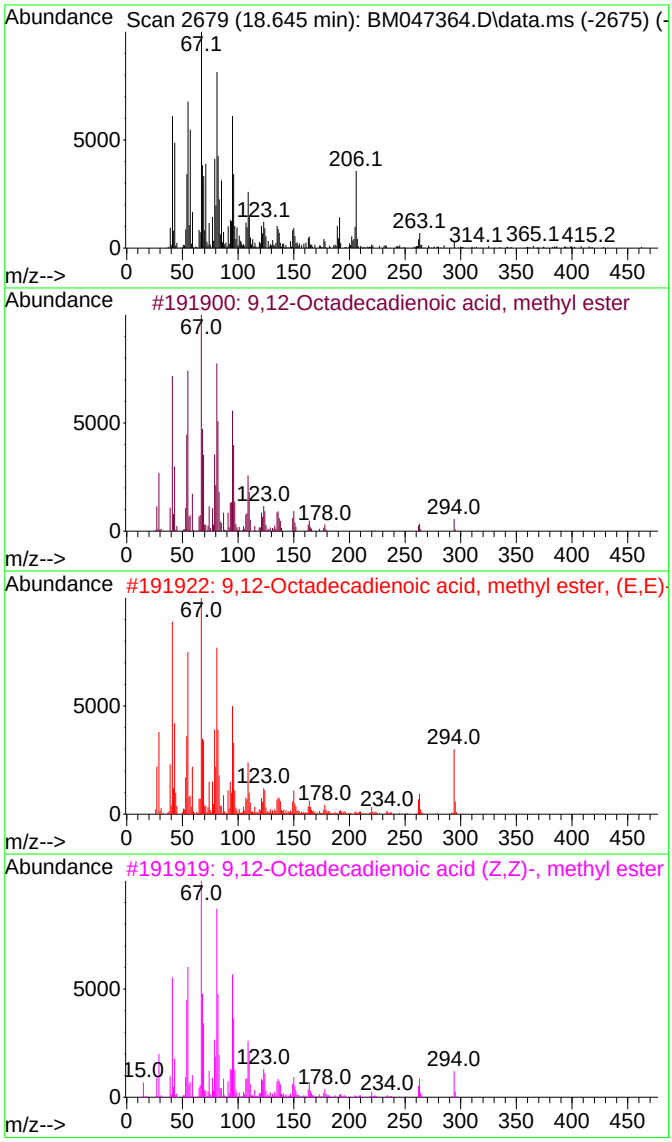
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

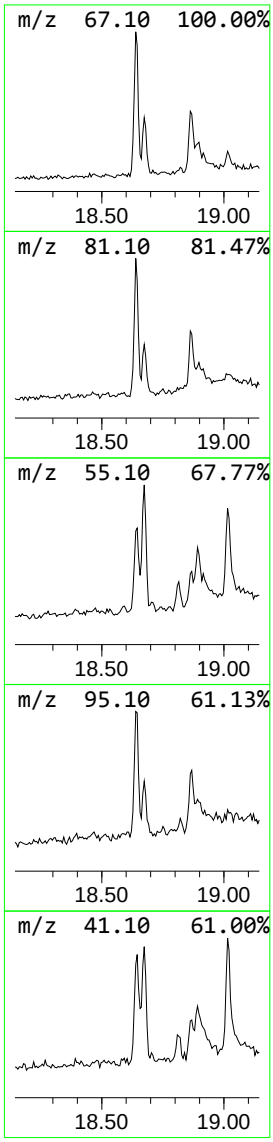
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 9,12-Octadecadienoic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.645	3.83 ng	733288	Phenanthrene-d10	16.780

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	98
4	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	97
5	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	97





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Data File : BM047364.D
Acq On : 27 Aug 2024 15:17
Operator : RC/JU
Sample : P3741-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TR-05-08262024

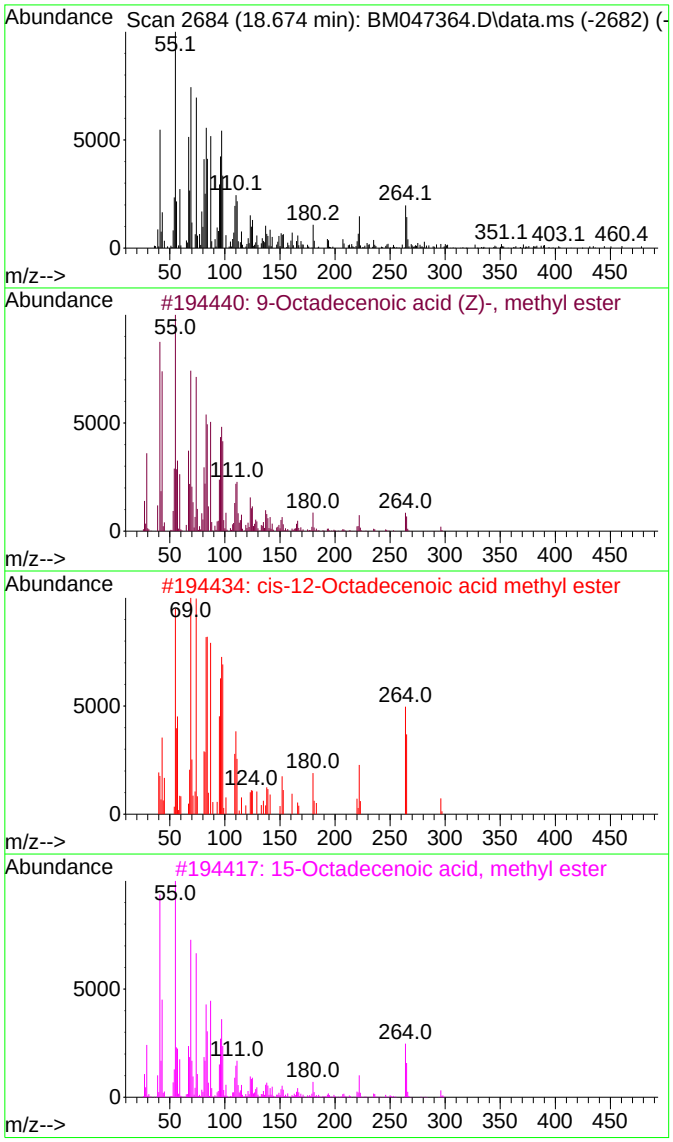
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

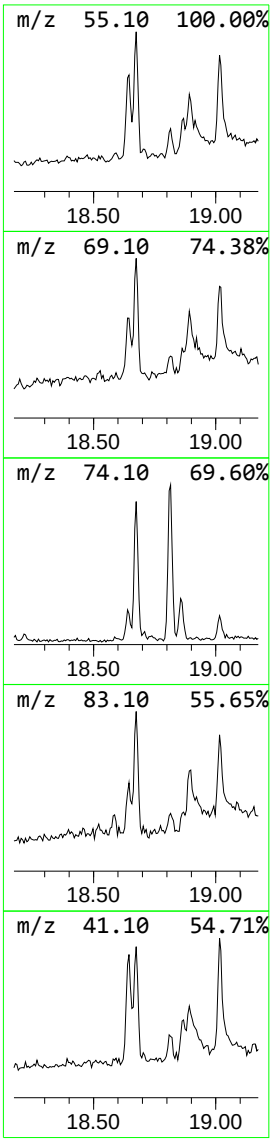
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 9-Octadecenoic acid (Z)-, m... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.674	2.74 ng	524674	Phenanthrene-d10	16.780

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	cis-12-Octadecenoic acid methyl ...	296	C19H36O2	1000427-68-4	99
3	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
4	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99
5	8-Octadecenoic acid, methyl este...	296	C19H36O2	026528-50-7	99





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Data File : BM047364.D
Acq On : 27 Aug 2024 15:17
Operator : RC/JU
Sample : P3741-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TR-05-08262024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.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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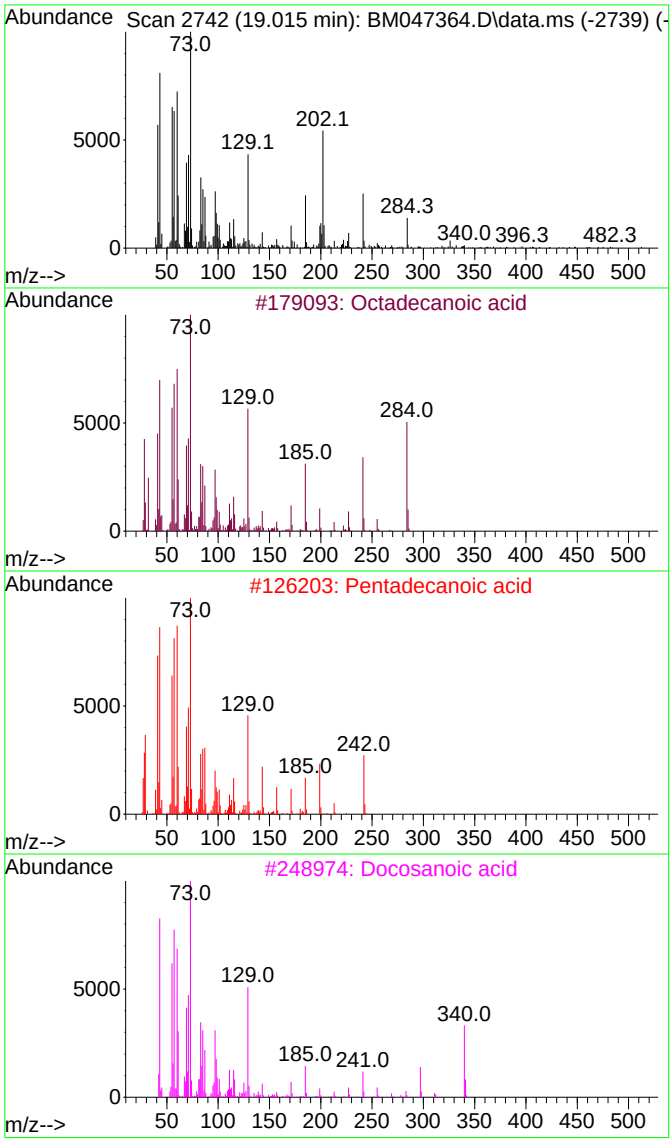
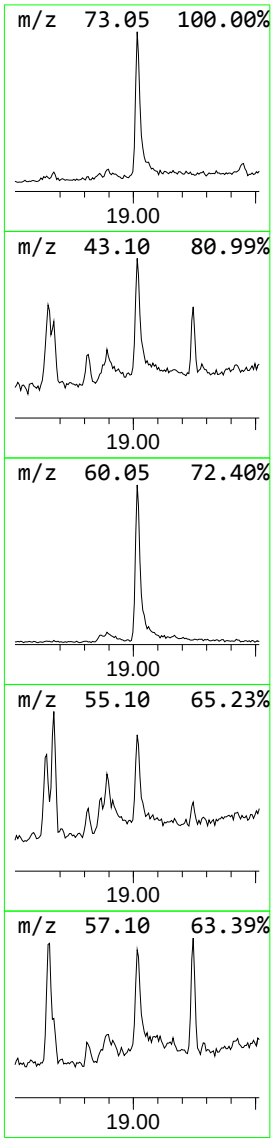
Peak Number 10 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.015	3.96 ng	566927	Chrysene-d12	21.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	78
3	Docosanoic acid	340	C22H44O2	000112-85-6	70
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082724\
Data File : BM047364.D
Acq On : 27 Aug 2024 15:17
Operator : RC/JU
Sample : P3741-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TR-05-08262024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.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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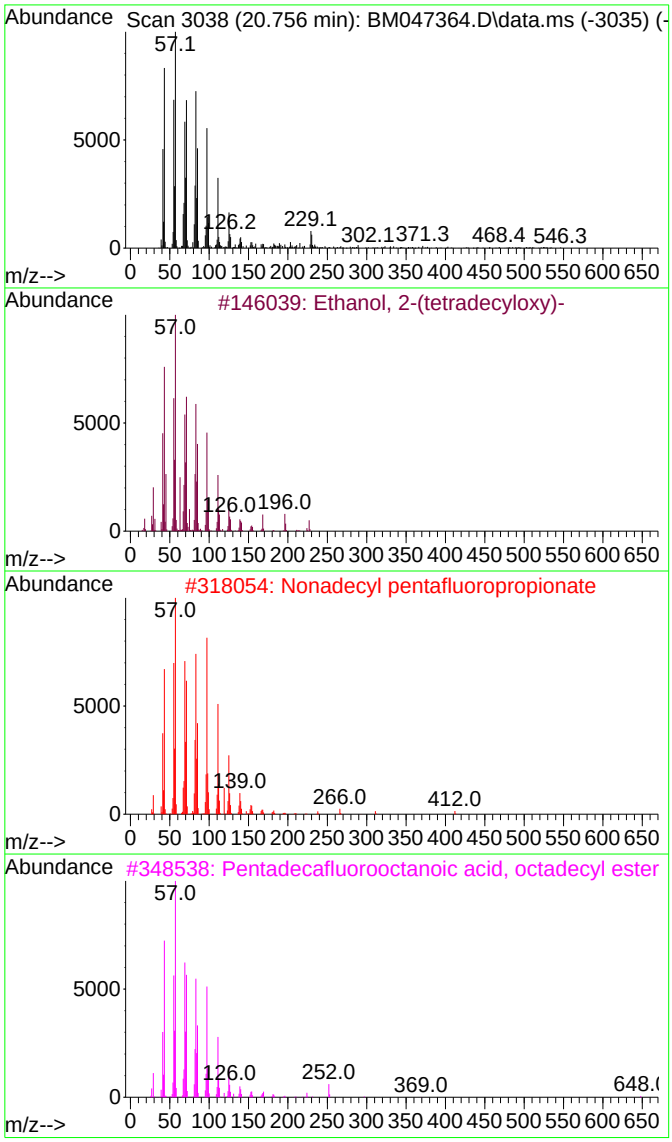
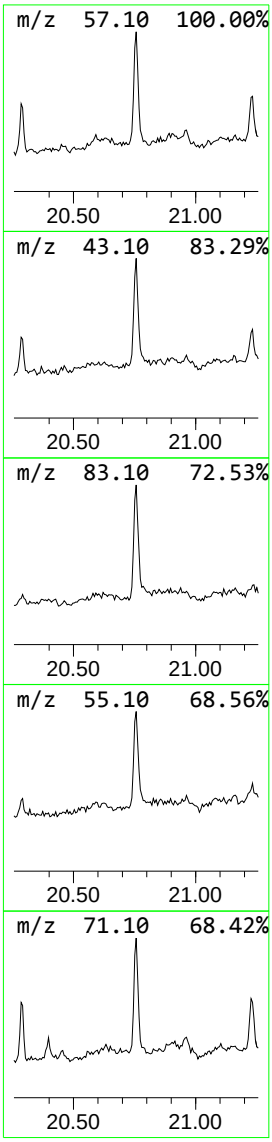
Peak Number 11 Ethanol, 2-(tetradecyloxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.756	4.02 ng	575699	Chrysene-d12	21.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
2	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	83
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	76
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082724\
Data File : BM047364.D
Acq On : 27 Aug 2024 15:17
Operator : RC/JU
Sample : P3741-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TR-05-08262024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.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
Propylene Glycol	3.257	3.2	ng	270838	1	7.351	1694570	20.0
2-Pentanone, 4-...	4.563	3.1	ng	259460	1	7.351	1694570	20.0
Ethanol, 2-(2-e...	6.981	2.3	ng	198424	1	7.351	1694570	20.0
1-Phenoxypropan...	10.869	3.6	ng	425058	2	10.104	2362720	20.0
unknown14.245	14.245	9.7	ng	1577100	3	14.010	3267060	20.0
unknown14.268	14.268	8.8	ng	1445720	3	14.010	3267060	20.0
n-Hexadecanoic ...	17.715	8.8	ng	1674800	4	16.780	3827420	20.0
9,12-Octadecadi...	18.645	3.8	ng	733288	4	16.780	3827420	20.0
9-Octadecenoic ...	18.674	2.7	ng	524674	4	16.780	3827420	20.0
Octadecanoic acid	19.015	4.0	ng	566927	5	21.027	2860960	20.0
Ethanol, 2-(tet...	20.756	4.0	ng	575699	5	21.027	2860960	20.0