LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091322\
Data File : BP011688.D
Acq On : 13 Sep 2022 16:34
Operator : CG/JU
Sample : N4557-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP-303-20220908

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-BP091322.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP011688.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.087	13	17	44	rVB	17648597	26138637	72.78%	13.907%
2	5.052	343	351	358	rBV	380804	569668	1.59%	0.303%
3	5.510	419	429	440	rBV	6078837	9211481	25.65%	4.901%
4	7.110	693	701	720	rBV	3556642	5676494	15.81%	3.020%
5	7.957	837	845	856	rBV	2137159	3396472	9.46%	1.807%
6	9.122	1033	1043	1055	rBV	7472123	12751856	35.50%	6.785%
7	9.263	1055	1067	1082	rVV	526897	1112723	3.10%	0.592%
8	10.769	1314	1323	1336	rBV	2835750	4826399	13.44%	2.568%
9	13.228	1732	1741	1752	rBV	18007617	27482181	76.52%	14.622%
10	14.598	1966	1974	1987	rBV	4118197	6102912	16.99%	3.247%
11	16.086	2220	2227	2246	rVB	13330099	19291387	53.71%	10.264%
12	17.351	2435	2442	2449	rBV	4933738	6992225	19.47%	3.720%
13	17.851	2522	2527	2532	rBV	356734	440048	1.23%	0.234%
14	18.233	2587	2592	2608	rBV2	1426417	2371418	6.60%	1.262%
15	18.521	2636	2641	2643	rBV	420310	631032	1.76%	0.336%
16	19.127	2740	2744	2750	rBV	309600	469990	1.31%	0.250%
17	19.463	2796	2801	2812	rBV	1174908	1911649	5.32%	1.017%
18	19.845	2860	2866	2871	rBV	859978	1586243	4.42%	0.844%
19	19.904	2871	2876	2881	rVB	27280132	35915702	100.00%	19.109%
20	20.768	3018	3023	3031	rBV	912177	1600003	4.45%	0.851%
21	21.433	3130	3136	3144	rVB	5580594	7415202	20.65%	3.945%
22	21.557	3152	3157	3172	rBV2	2596427	4764534	13.27%	2.535%
23	23.898	3548	3555	3568	rVB	3548237	7293767	20.31%	3.881%

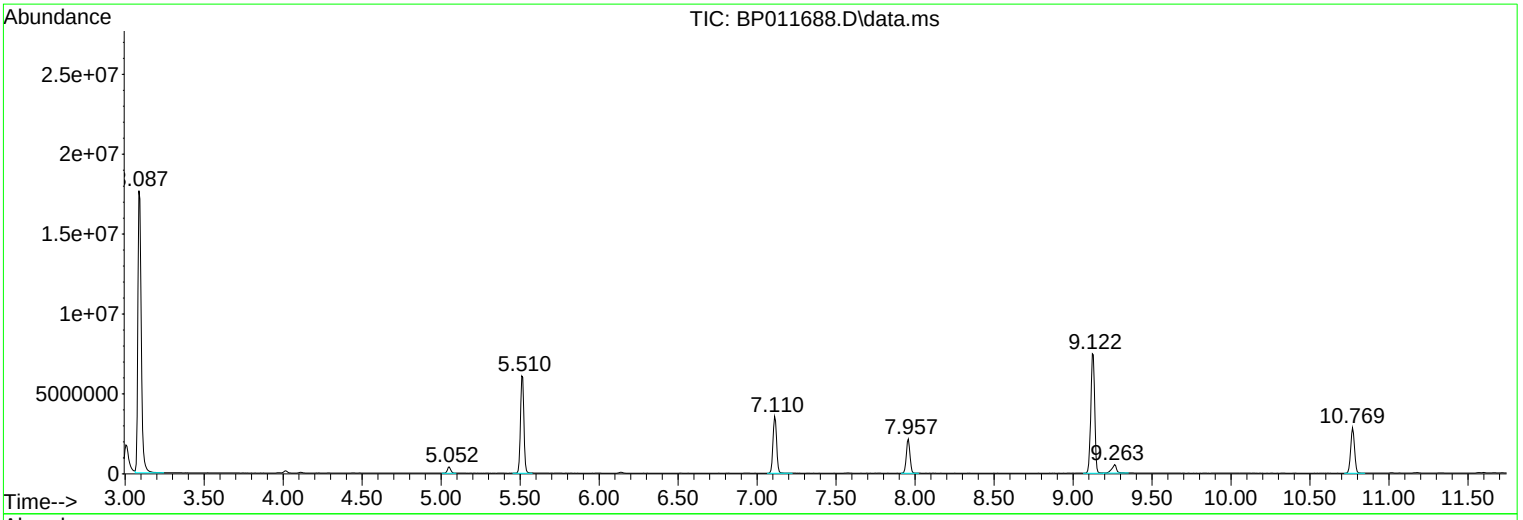
Sum of corrected areas: 187952023

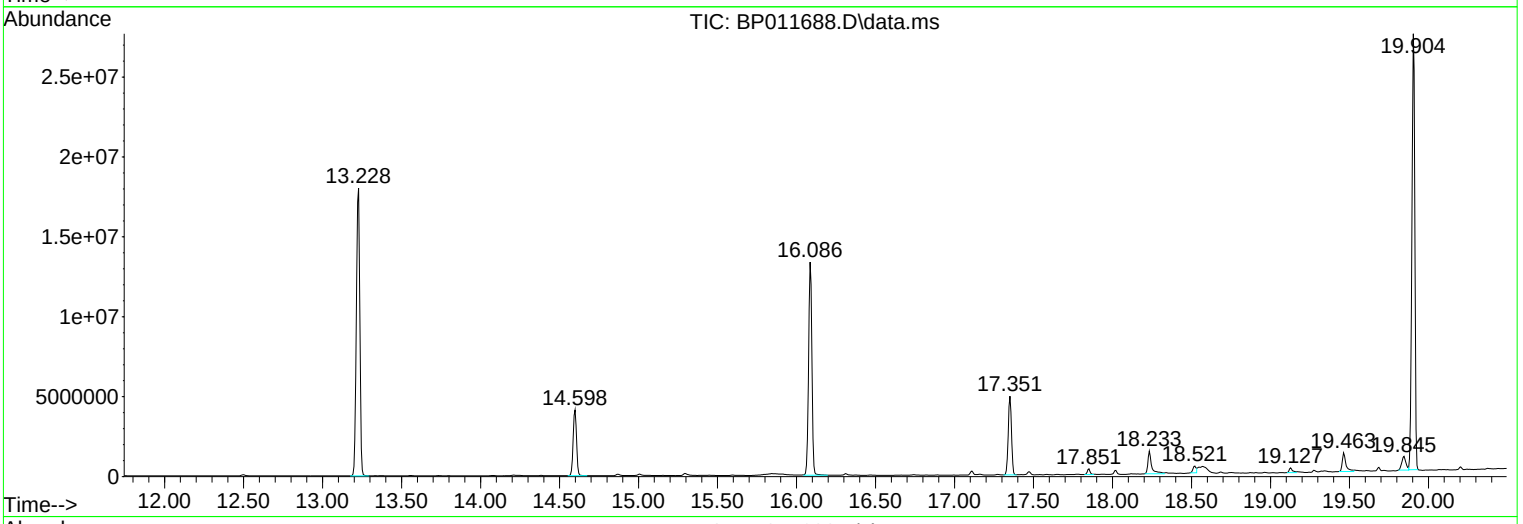
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091322\
Data File : BP011688.D
Acq On : 13 Sep 2022 16:34
Operator : CG/JU
Sample : N4557-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

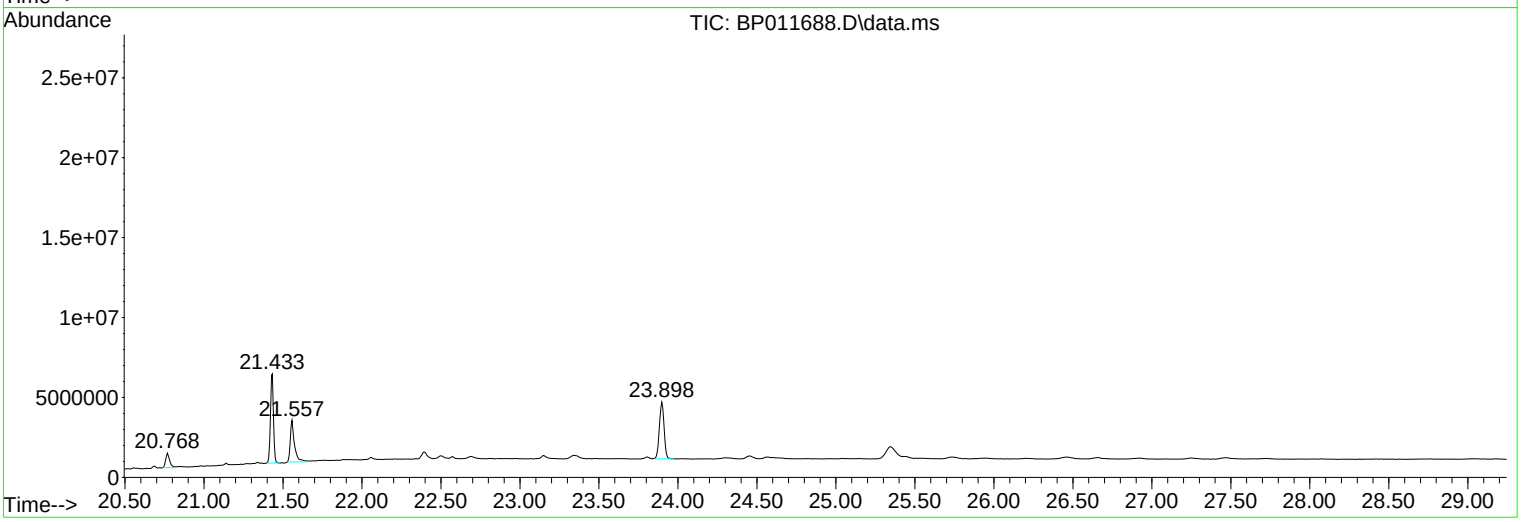
Instrument :
BNA_P
ClientSampleId :
SP-303-20220908

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091322.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\BP091322\
Data File : BP011688.D
Acq On : 13 Sep 2022 16:34
Operator : CG/JU
Sample : N4557-03
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Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

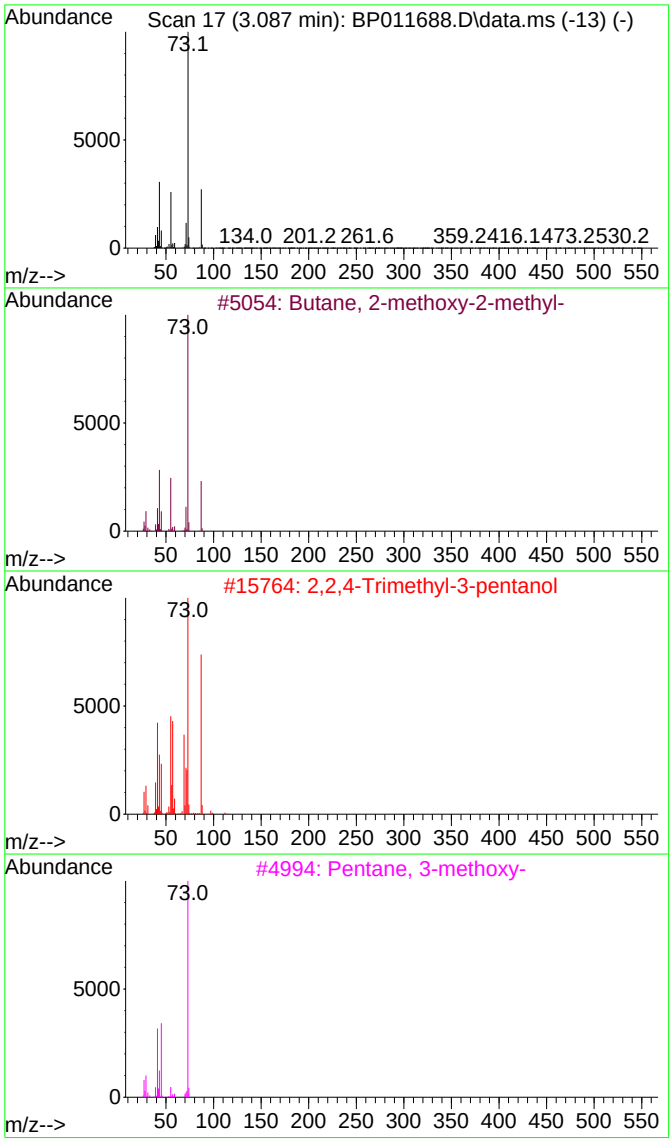
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

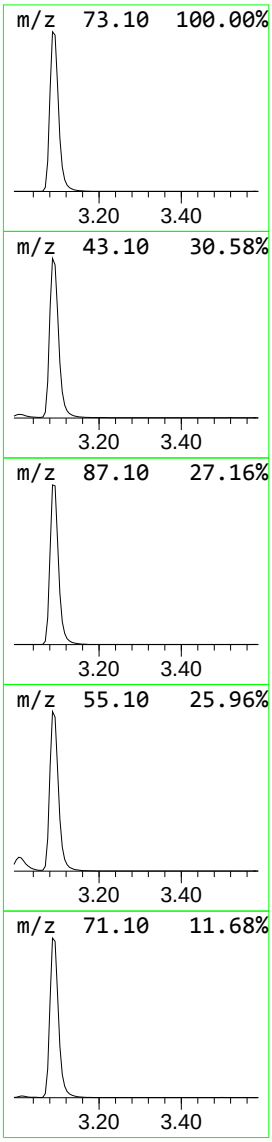
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.087	153.92 ng	26138600	1,4-Dichlorobenzene-d4	7.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091322\
Data File : BP011688.D
Acq On : 13 Sep 2022 16:34
Operator : CG/JU
Sample : N4557-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP-303-20220908

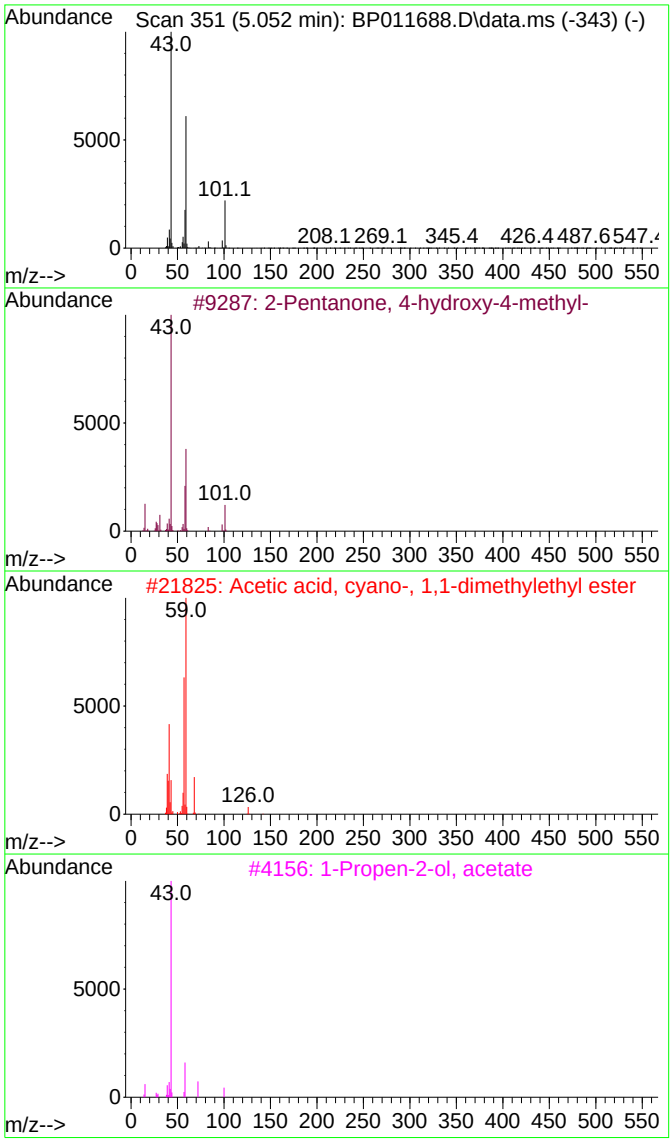
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

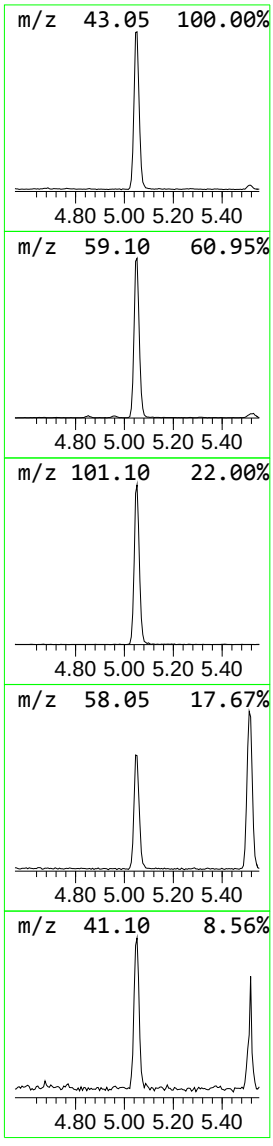
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.052	3.35 ng	569668	1,4-Dichlorobenzene-d4	7.957

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	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Acetone	58	C3H6O	000067-64-1	9





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Data File : BP011688.D
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Sample : N4557-03
Misc :
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Instrument :
BNA_P
ClientSampleId :
SP-303-20220908

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

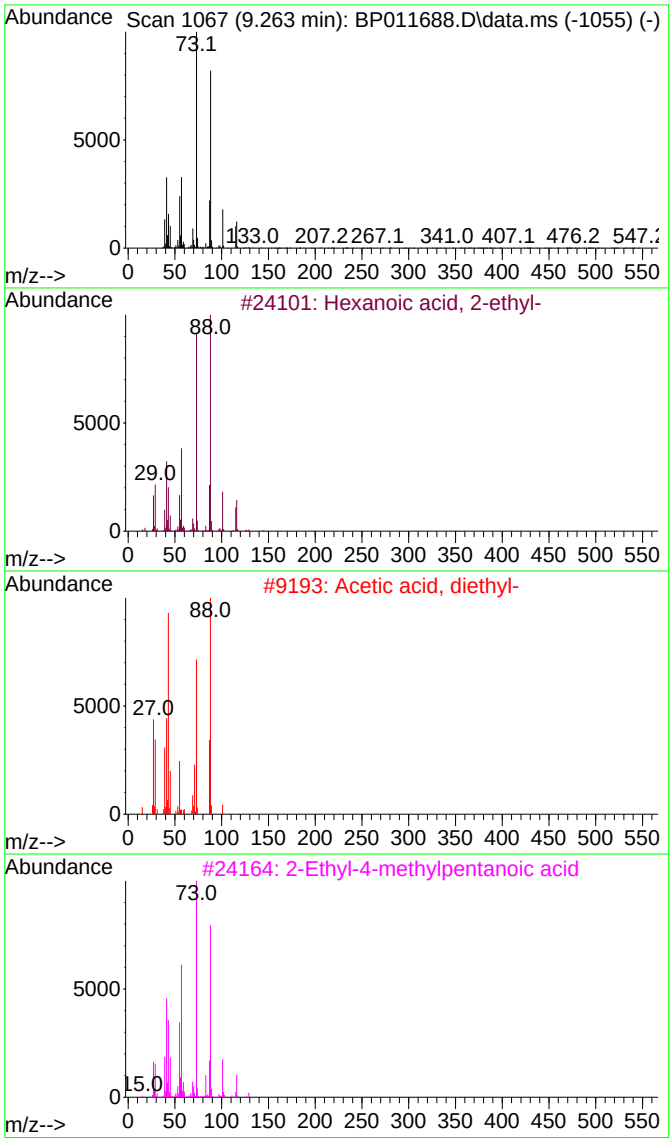
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

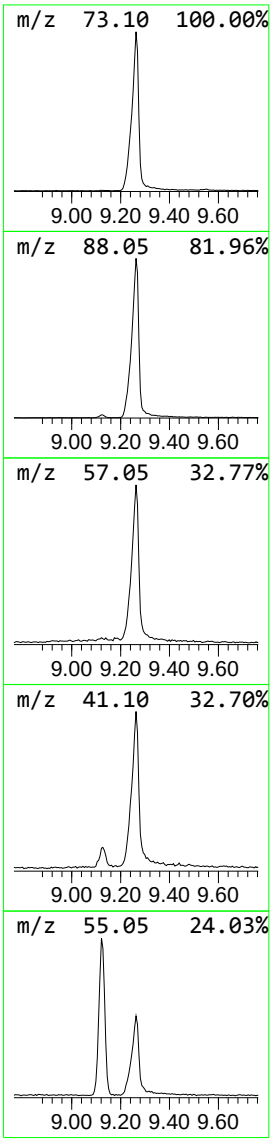
****

Peak Number 3 Hexanoic acid, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.263	6.55 ng	1112720	1,4-Dichlorobenzene-d4	7.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
2	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	59
3	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	56
4	Diisopropanolamine	133	C6H15NO2	000110-97-4	43
5	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091322\
Data File : BP011688.D
Acq On : 13 Sep 2022 16:34
Operator : CG/JU
Sample : N4557-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP-303-20220908

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

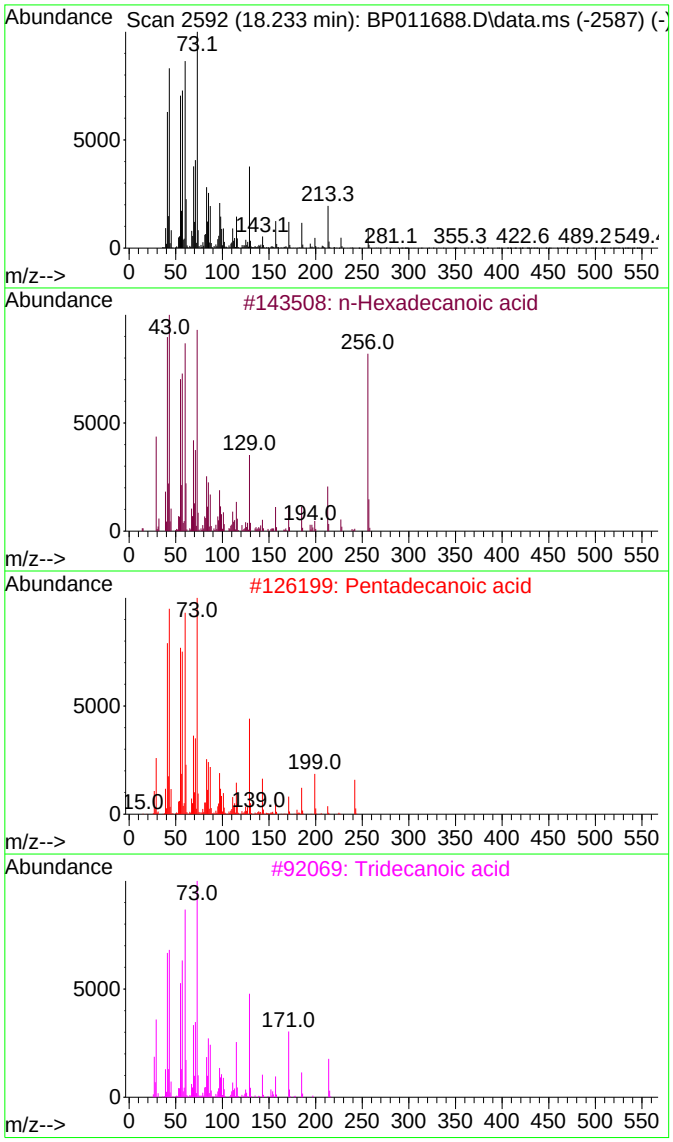
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

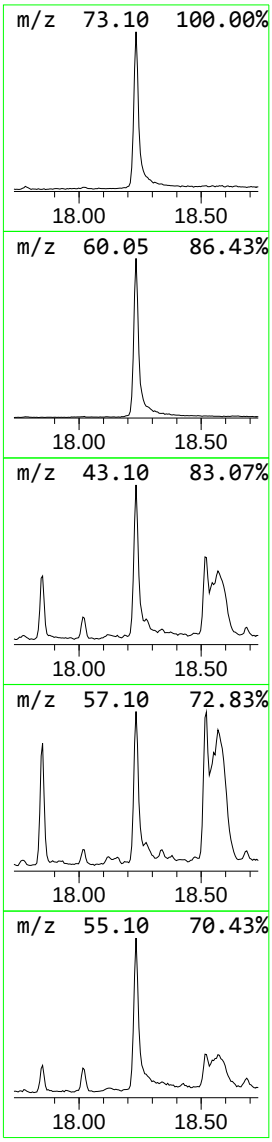
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.233	6.78 ng	2371420	Phenanthrene-d10	17.351

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	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	92
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091322\
Data File : BP011688.D
Acq On : 13 Sep 2022 16:34
Operator : CG/JU
Sample : N4557-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP-303-20220908

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

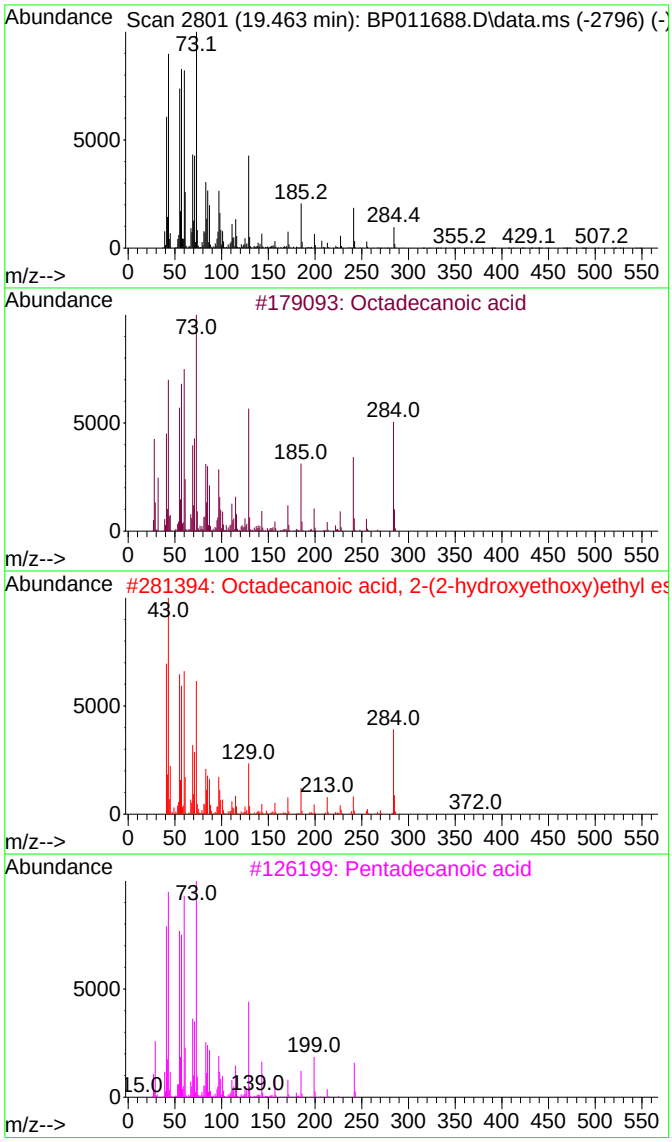
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

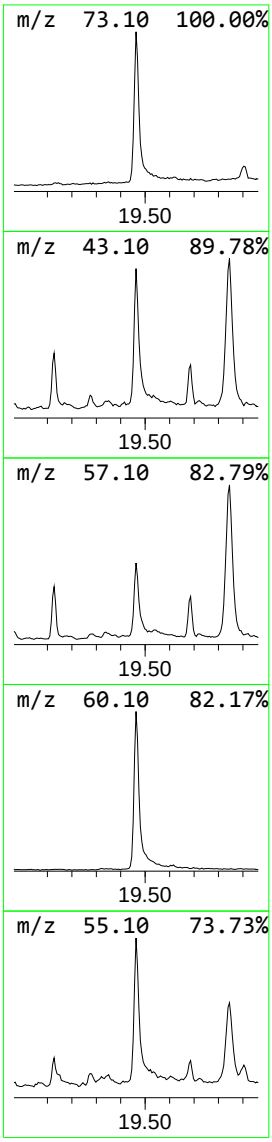
****

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.463	5.16 ng	1911650	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091322\
Data File : BP011688.D
Acq On : 13 Sep 2022 16:34
Operator : CG/JU
Sample : N4557-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP-303-20220908

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

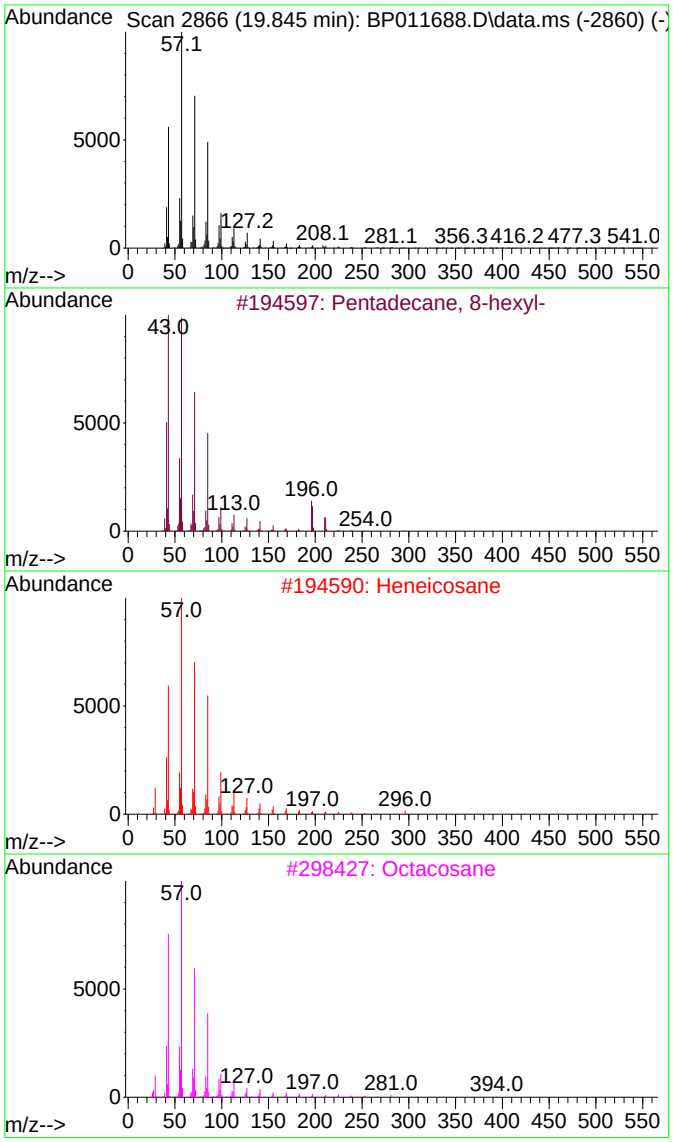
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

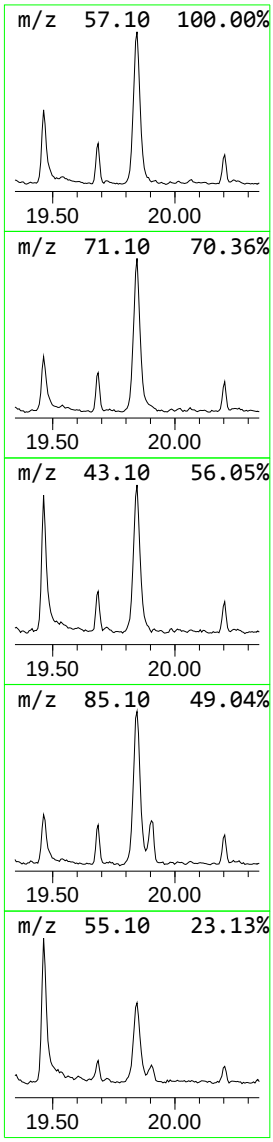
****

Peak Number 6 Pentadecane, 8-hexyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.845	4.28 ng	1586240	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091322\
Data File : BP011688.D
Acq On : 13 Sep 2022 16:34
Operator : CG/JU
Sample : N4557-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP-303-20220908

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

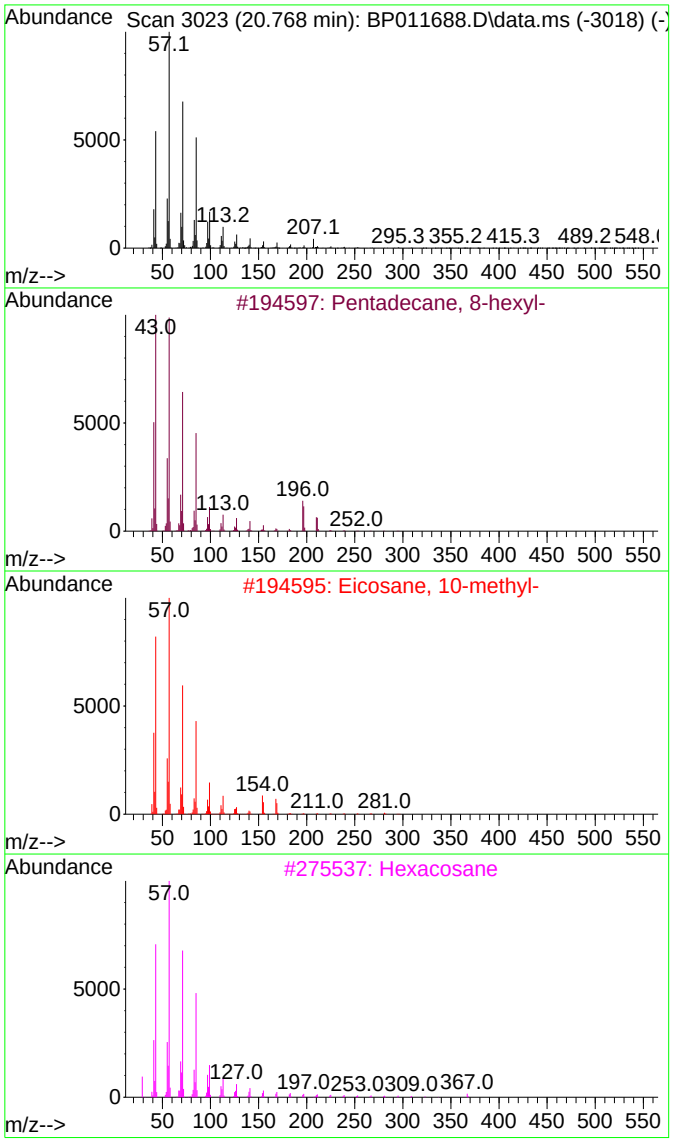
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

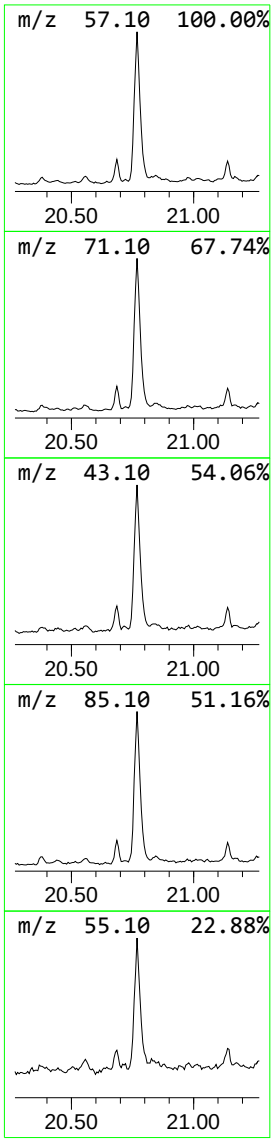
****

Peak Number 7 Eicosane, 10-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.768	4.32 ng	1600000	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
3	Hexacosane	366	C26H54	000630-01-3	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Heptacosane	380	C27H56	000593-49-7	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091322\
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Sample : N4557-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

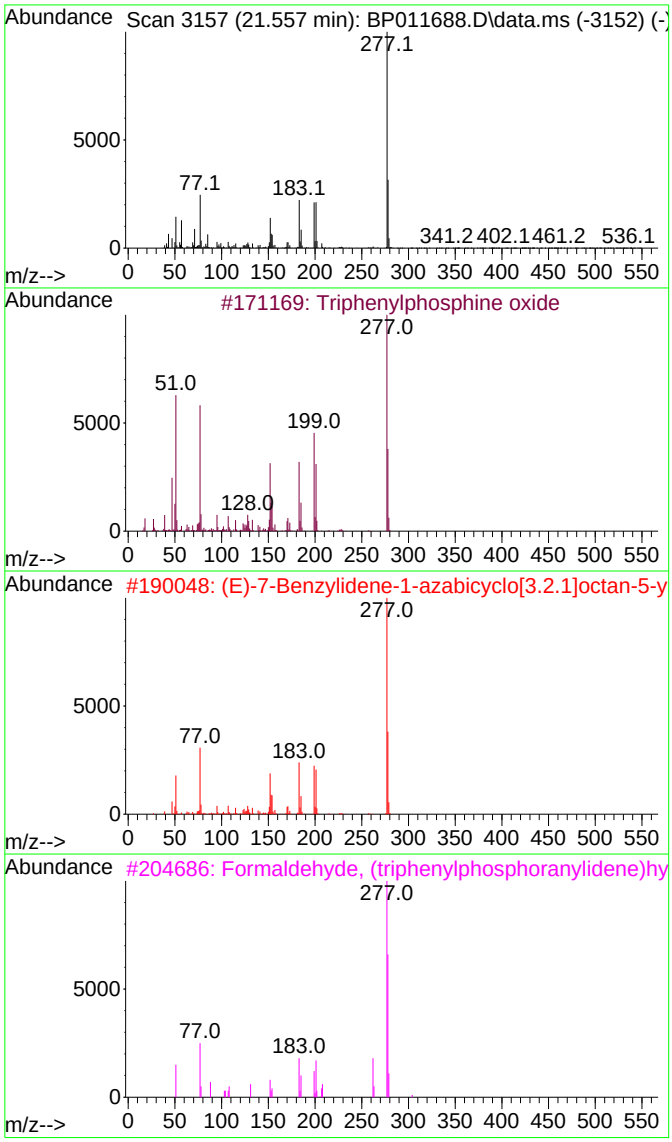
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

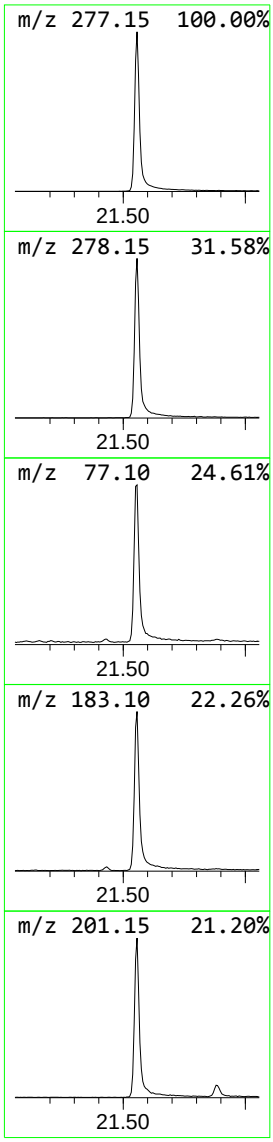
****

Peak Number 8 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.557	12.85 ng	4764530	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	91
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	38
5	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091322\
Data File : BP011688.D
Acq On : 13 Sep 2022 16:34
Operator : CG/JU
Sample : N4557-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP-303-20220908

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091322.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
Butane, 2-metho...	3.087	153.9	ng	26138600	1	7.957	3396470	20.0
2-Pentanone, 4-...	5.052	3.4	ng	569668	1	7.957	3396470	20.0
Hexanoic acid, ...	9.263	6.5	ng	1112720	1	7.957	3396470	20.0
n-Hexadecanoic ...	18.233	6.8	ng	2371420	4	17.351	6992230	20.0
Octadecanoic acid	19.463	5.2	ng	1911650	5	21.433	7415200	20.0
Pentadecane, 8-...	19.845	4.3	ng	1586240	5	21.433	7415200	20.0
Eicosane, 10-me...	20.768	4.3	ng	1600000	5	21.433	7415200	20.0
Triphenylphosph...	21.557	12.9	ng	4764530	5	21.433	7415200	20.0