LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052522\
Data File : BF128464.D
Acq On : 25 May 2022 17:23
Operator : CG\JU
Sample : N2896-16
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P039-SS001-2430-01

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_F\Methods\8270-BF052022.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128464.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.445	534	537	557	rBV	1993620	2157019	59.87%	10.127%
2	6.004	629	632	637	rBV	52067	47687	1.32%	0.224%
3	6.116	647	651	658	rBV	686056	546497	15.17%	2.566%
4	6.469	707	711	724	rBV	1774599	2159859	59.95%	10.140%
5	6.810	765	769	775	rVB	616397	547589	15.20%	2.571%
6	7.381	861	866	869	rBV	1378309	1356039	37.64%	6.366%
7	8.092	983	987	992	rBV	741838	640102	17.77%	3.005%
8	9.169	1165	1170	1173	rBV	2262534	1993057	55.32%	9.357%
9	9.845	1281	1285	1289	rBV	711228	616289	17.11%	2.893%
10	10.639	1417	1420	1435	rBV	1105970	1101163	30.57%	5.170%
11	11.339	1535	1539	1542	rBV	710413	578529	16.06%	2.716%
12	11.857	1619	1627	1631	rBV2	101575	143721	3.99%	0.675%
13	11.892	1631	1633	1636	rVB	179112	138667	3.85%	0.651%
14	12.557	1742	1746	1750	rBV	217009	190733	5.29%	0.895%
15	12.786	1779	1785	1788	rBV	204202	206762	5.74%	0.971%
16	12.810	1788	1789	1797	rVB3	30772	61483	1.71%	0.289%
17	12.927	1805	1809	1812	rVB	1826627	1560411	43.31%	7.326%
18	13.486	1901	1904	1906	rBV2	39338	43669	1.21%	0.205%
19	13.798	1954	1957	1962	rBV3	77681	114078	3.17%	0.536%
20	13.845	1962	1965	1974	rBV2	59101	128442	3.57%	0.603%
21	13.957	1980	1984	1987	rBV	3574175	3602635	100.00%	16.914%
22	13.992	1987	1990	1993	rVB	439405	429160	11.91%	2.015%
23	14.080	2003	2005	2010	rVB2	50310	49939	1.39%	0.234%
24	14.127	2010	2013	2016	rBV2	55663	55234	1.53%	0.259%
25	14.368	2050	2054	2058	rBV	265194	269890	7.49%	1.267%
26	14.433	2062	2065	2067	rVV2	52764	58690	1.63%	0.276%
27	14.468	2067	2071	2075	rVV2	525270	522647	14.51%	2.454%
28	14.521	2078	2080	2085	rVV4	52423	80658	2.24%	0.379%
29	14.568	2085	2088	2089	rVV2	368888	358115	9.94%	1.681%
30	14.586	2089	2091	2096	rVB	346155	307089	8.52%	1.442%
31	14.692	2103	2109	2114	rVB2	327632	515766	14.32%	2.421%
32	14.804	2124	2128	2136	rVB4	160588	354210	9.83%	1.663%
33	15.033	2165	2167	2170	rBV	49435	61584	1.71%	0.289%
34	15.462	2236	2240	2245	rVB	250696	302911	8.41%	1.422%

Sum of corrected areas: 21300324

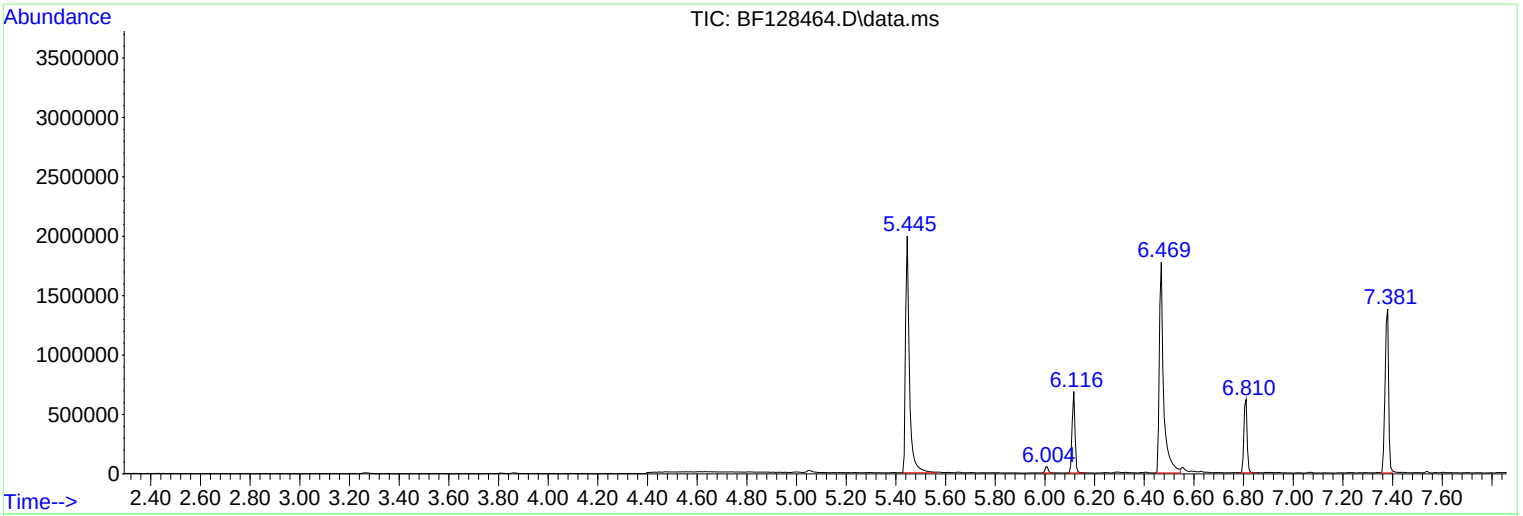
Instrument :
BNA_F
ClientSampleId :
P039-SS001-2430-01

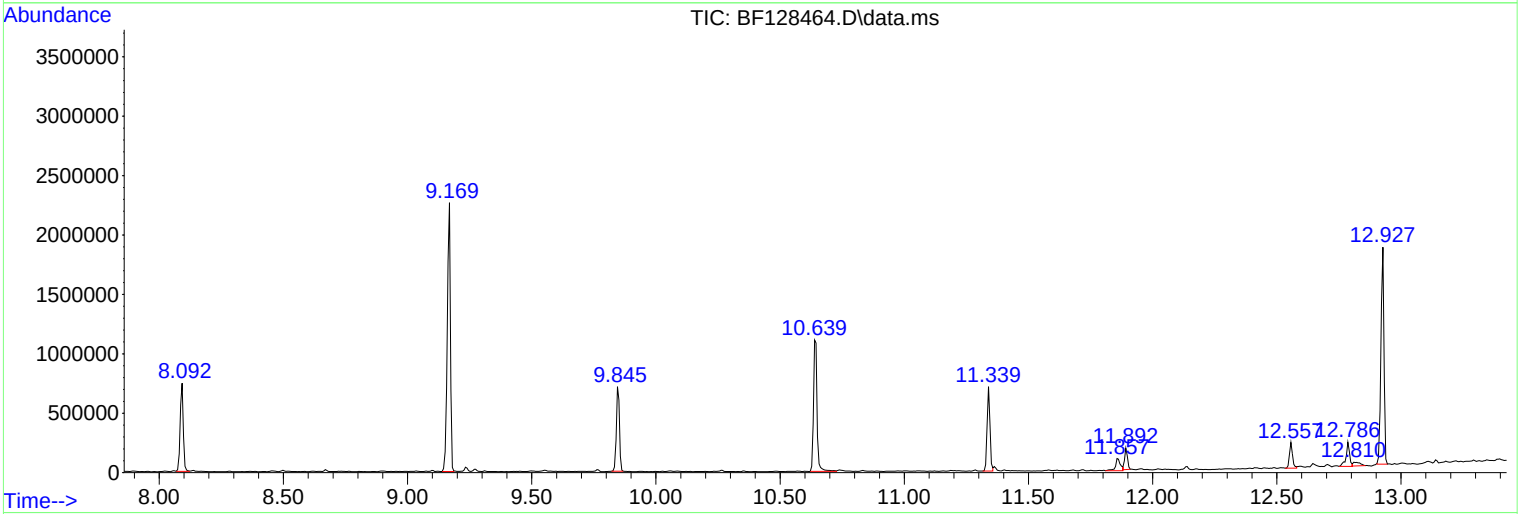
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052522\
Data File : BF128464.D
Acq On : 25 May 2022 17:23
Operator : CG\JU
Sample : N2896-16
Misc :
ALS Vial : 13 Sample Multiplier: 1

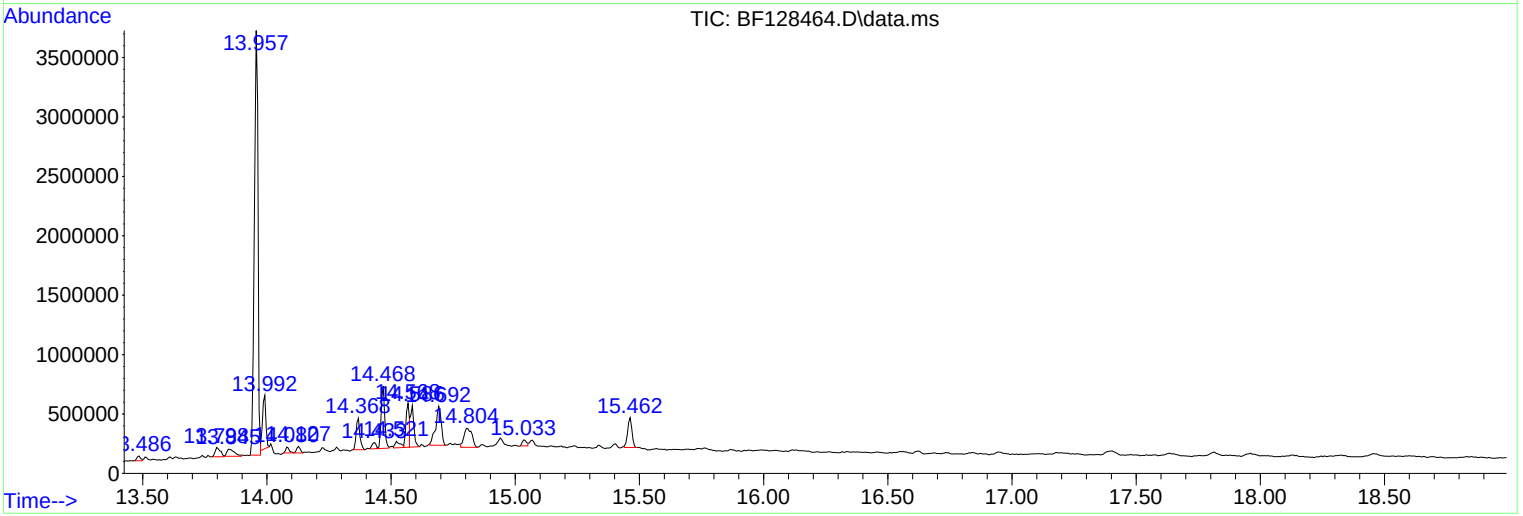
Instrument :
BNA_F
ClientSampleId :
P039-SS001-2430-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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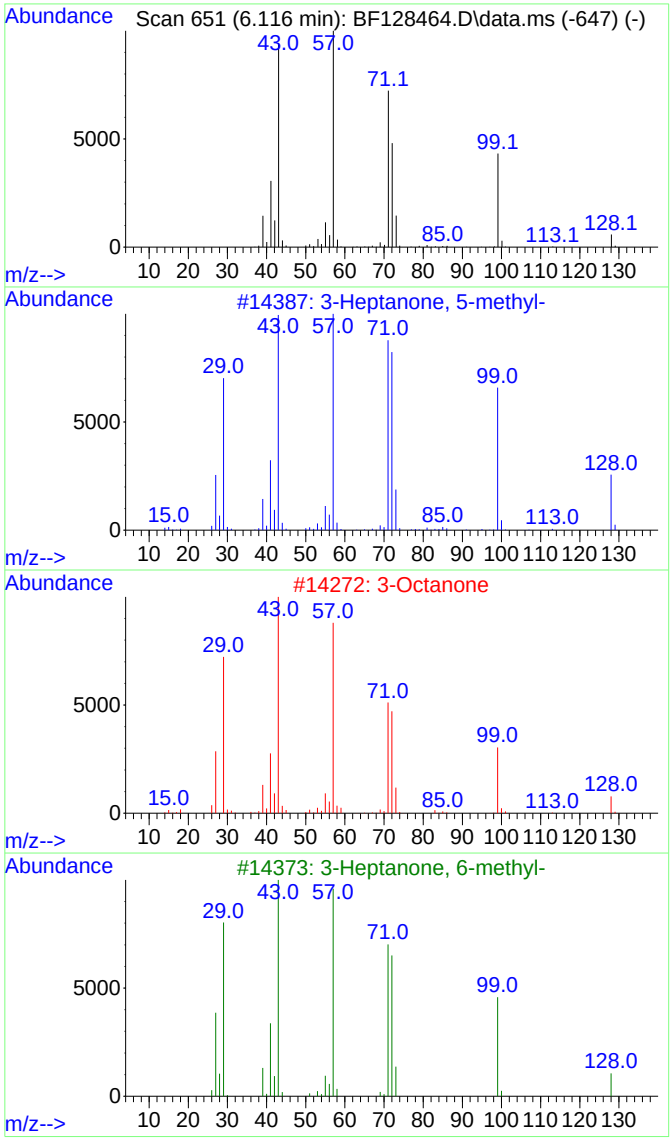
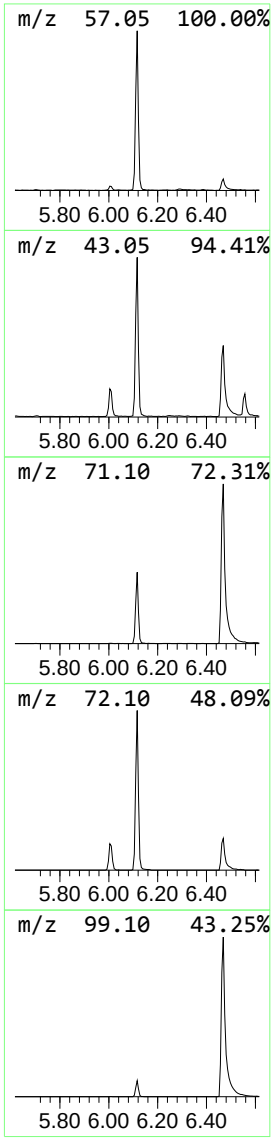
****

Peak Number 1 3-Heptanone, 5-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.116	19.96 ng	546497	1,4-Dichlorobenzene-d4	6.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	91
2	3-Octanone	128	C8H16O	000106-68-3	80
3	3-Heptanone, 6-methyl-	128	C8H16O	000624-42-0	59
4	2-Pentene, 5-(pentyloxy)-, (E)-	156	C10H20O	056052-85-8	43
5	3-Heptanone, 4-methyl-	128	C8H16O	006137-11-7	43





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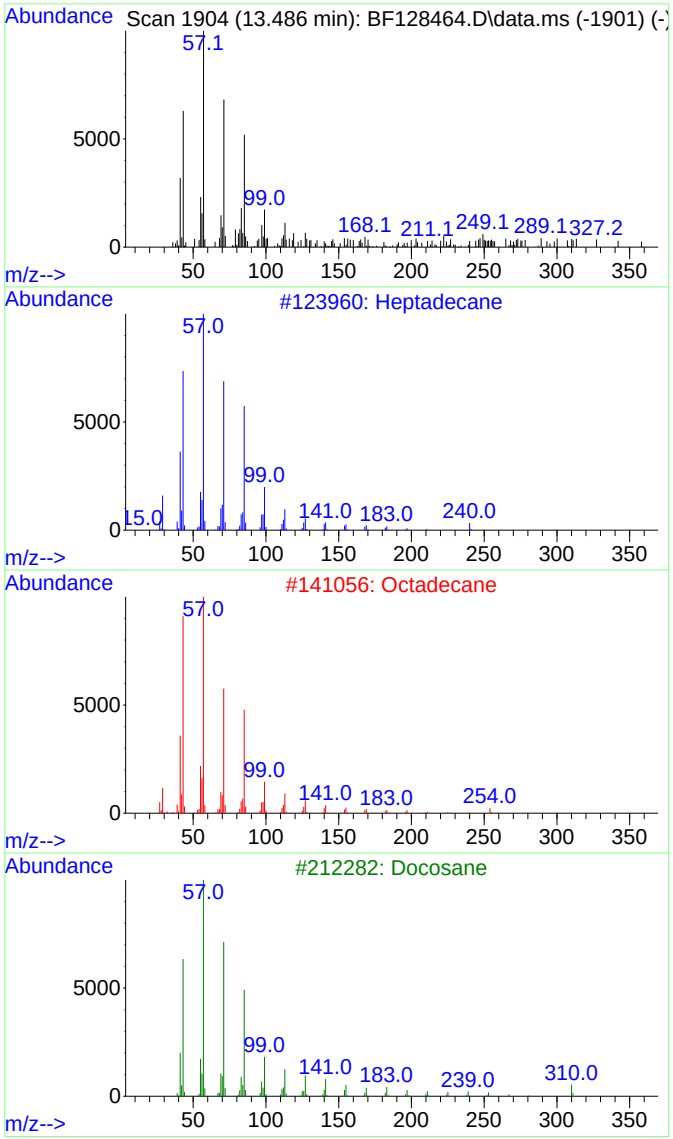
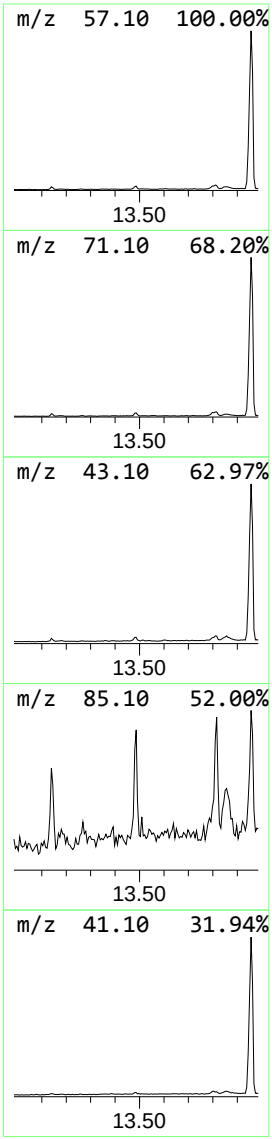
****

Peak Number 2 Heptadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.486	2.04 ng	43669	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Octadecane	254	C18H38	000593-45-3	91
3	Docosane	310	C22H46	000629-97-0	86
4	Nonadecane	268	C19H40	000629-92-5	83
5	Tetracosane	338	C24H50	000646-31-1	58





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Operator : CG\JU
Sample : N2896-16
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P039-SS001-2430-01

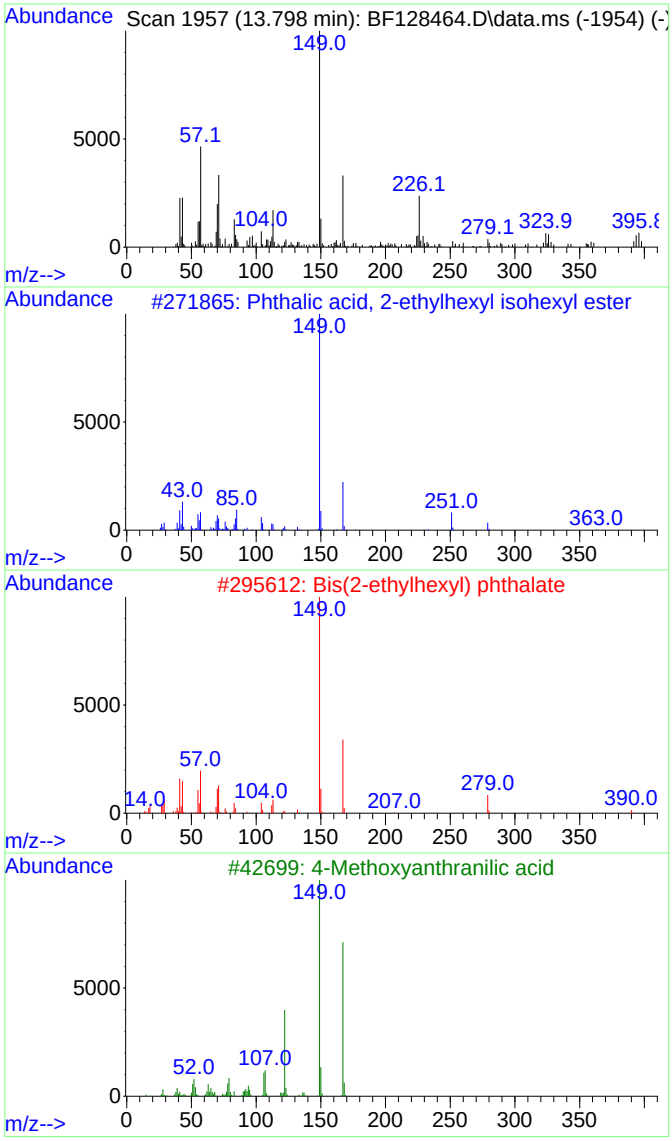
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

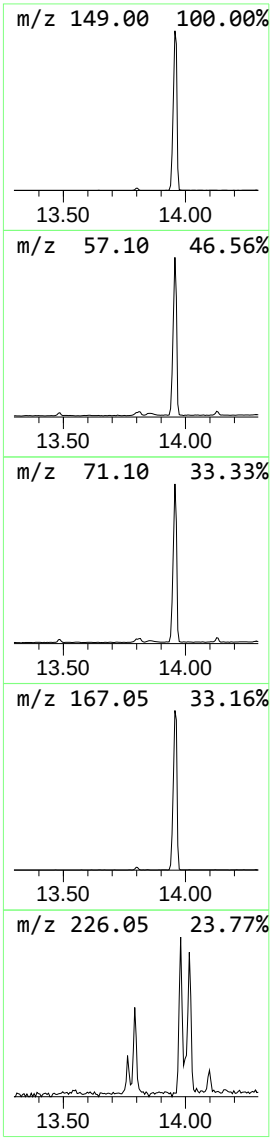
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Phthalic acid, 2-ethylhexyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.798	5.32 ng	114078	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, 2-ethylhexyl isoh...	362	C22H34O4	1000308-98-5	52
2	Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	52
3	4-Methoxyanthranilic acid	167	C8H9NO3	004294-95-5	52
4	Phthalic acid, di(hept-3-yl) ester	362	C22H34O4	1000357-00-0	50
5	Phthalic acid, hex-3-yl isohexyl...	334	C20H30O4	1000356-95-6	50





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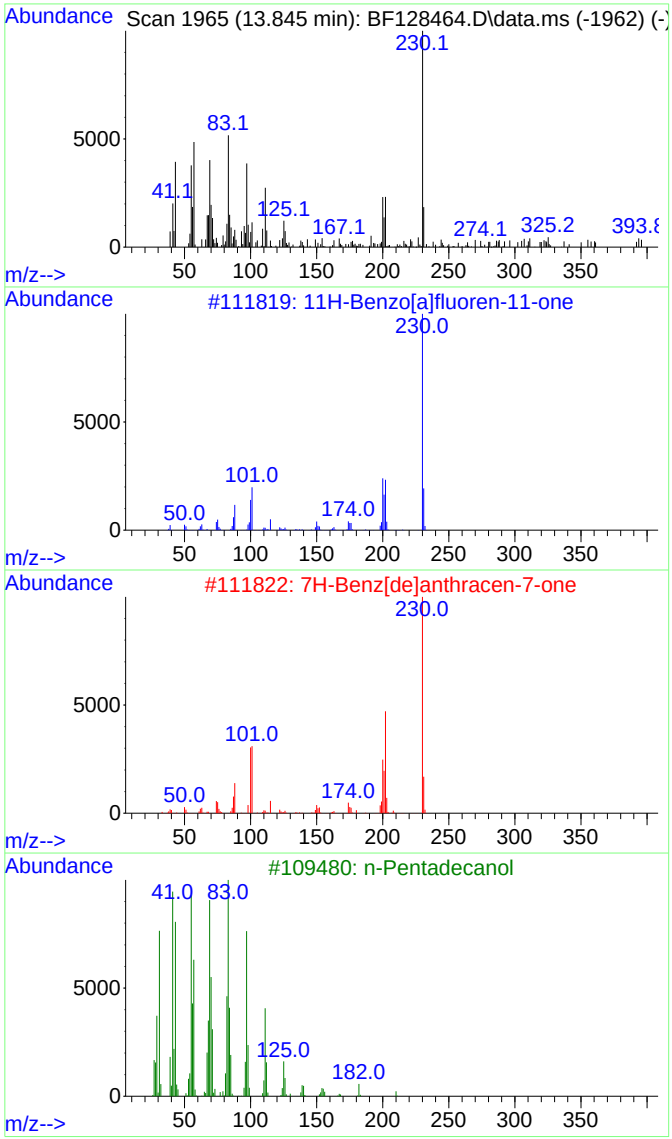
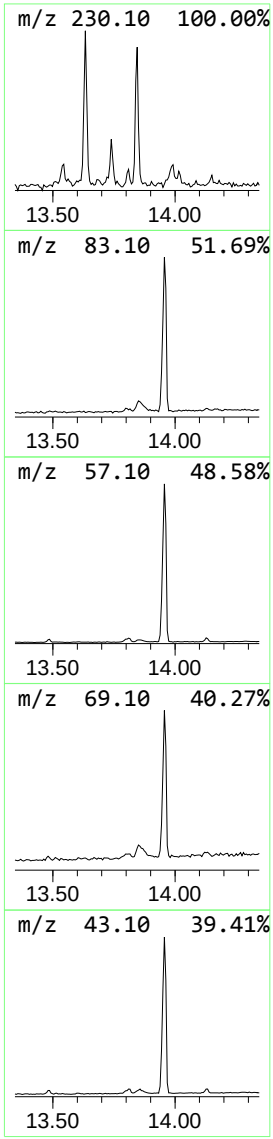
****

Peak Number 4 11H-Benzo[a]fluoren-11-one Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	5.99 ng	128442	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	64
2	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	46
3	n-Pentadecanol	228	C15H32O	000629-76-5	30
4	Visnagin	230	C13H10O4	000082-57-5	25
5	5-Amino-7-imino-4,8-diazatricycl...	230	C12H14N4O	1000388-35-6	22





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

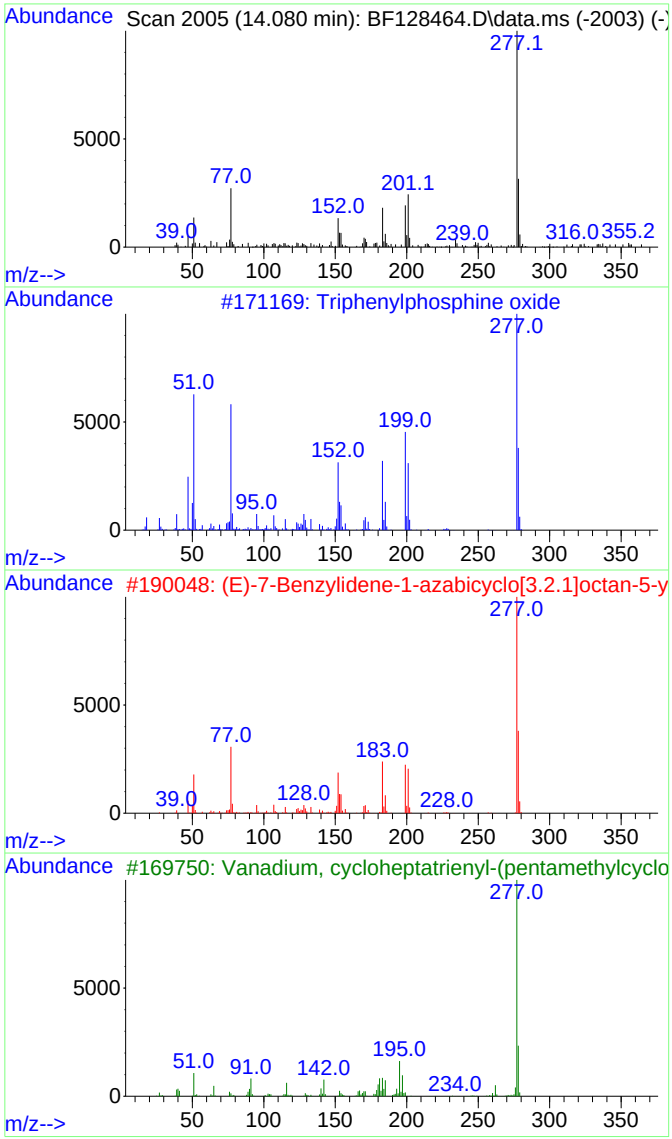
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

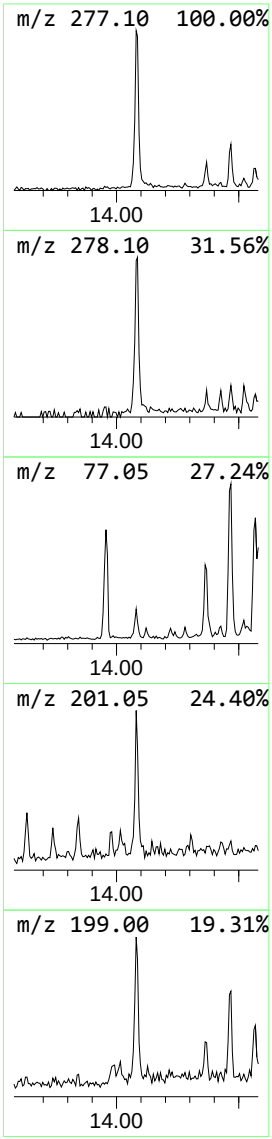
****

Peak Number 5 Triphenylphosphine oxide Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.080	2.33 ng	49939	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	87
3	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	47
4	4-Nitro-4'-methyldiphenylsulfone	277	C13H11NO4S	004094-37-5	43
5	Benzoic acid, 2-(diphenylphosphi...	306	C19H15O2P	017261-28-8	38





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Instrument :
BNA_F
ClientSampleId :
P039-SS001-2430-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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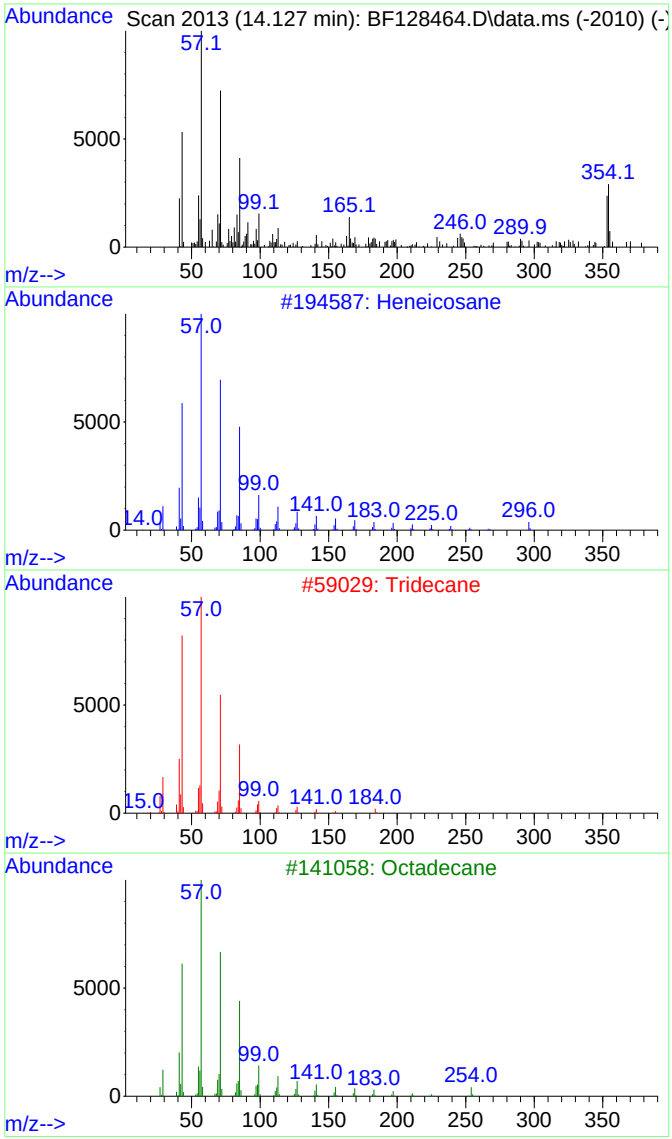
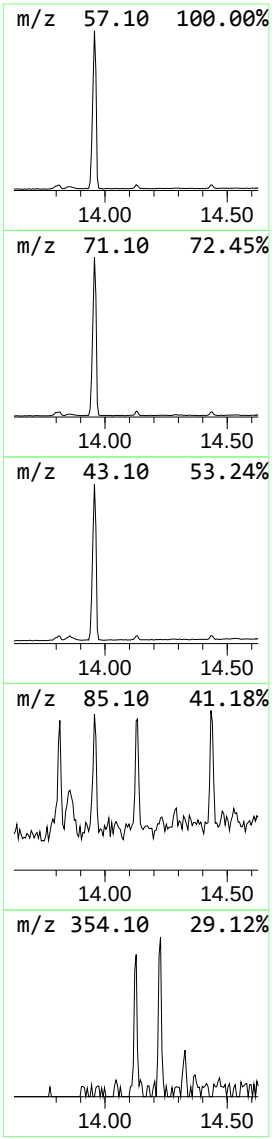
****

Peak Number 6 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.127	2.57 ng	55234	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	55
2	Tridecane	184	C13H28	000629-50-5	55
3	Octadecane	254	C18H38	000593-45-3	49
4	Docosane	310	C22H46	000629-97-0	46
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	46





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Operator : CG\JU
Sample : N2896-16
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P039-SS001-2430-01

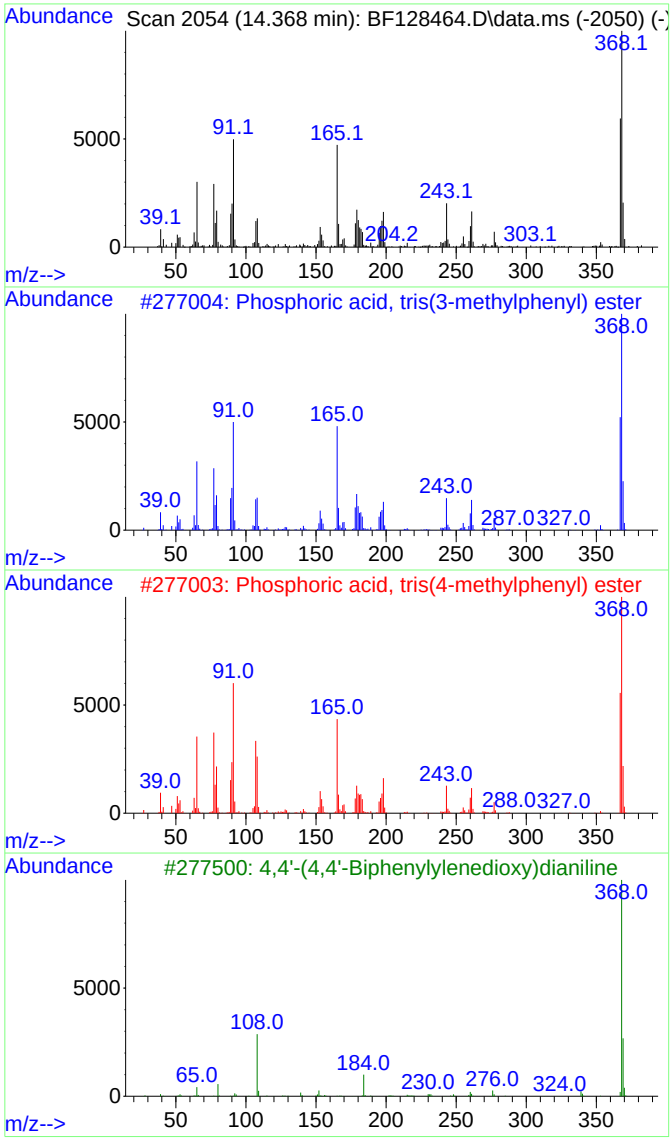
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

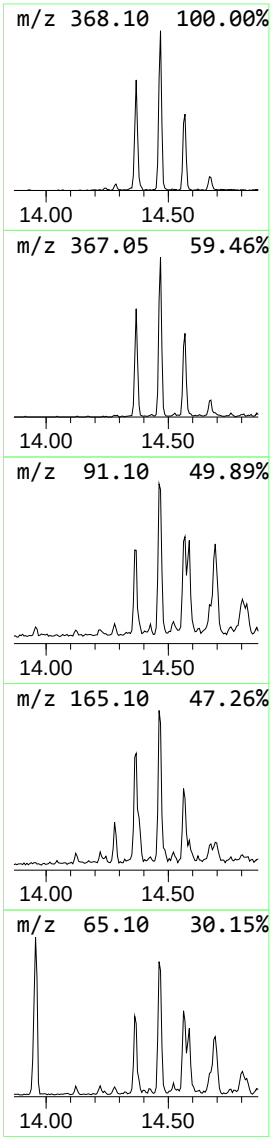
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Phosphoric acid, tris(4-met... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.368	12.58 ng	269890	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phosphoric acid, tris(3-methylph...	368	C21H21O4P	000563-04-2	99
2	Phosphoric acid, tris(4-methylph...	368	C21H21O4P	000078-32-0	94
3	4,4'-(4,4'-Biphenylylenedioxy)di...	368	C24H20N2O2	013080-85-8	27
4	Cholest-5-en-3-ol (3.beta.)-, 3-...	516	C36H52O2	001990-11-0	16
5	Cholesteryl benzoate	490	C34H50O2	000604-32-0	16





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BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

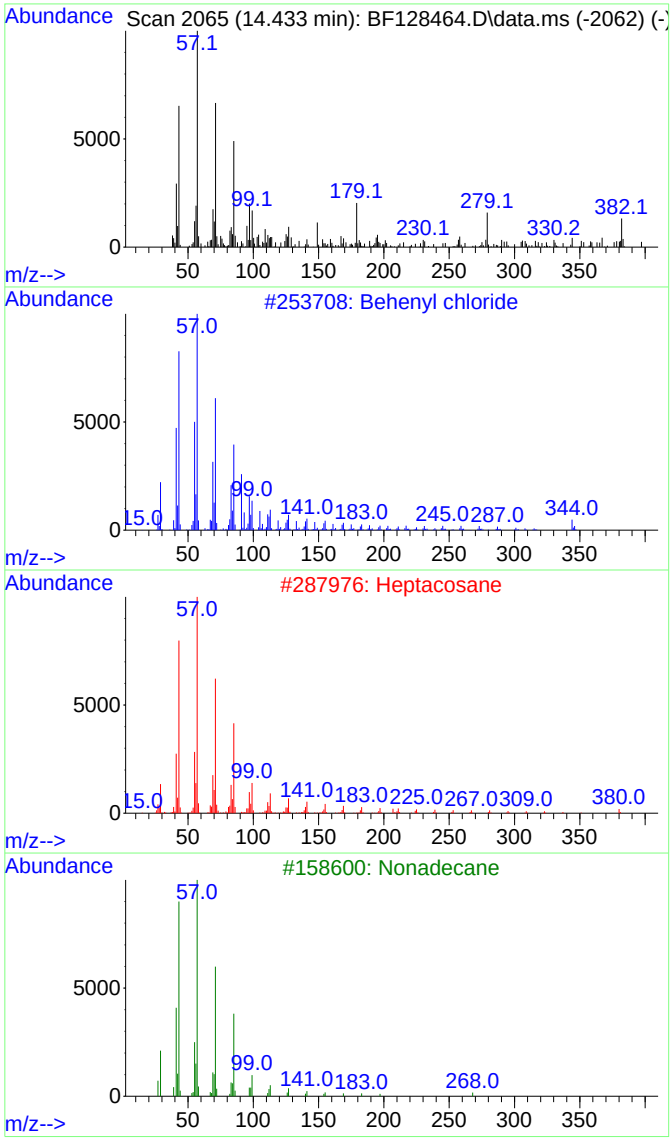
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

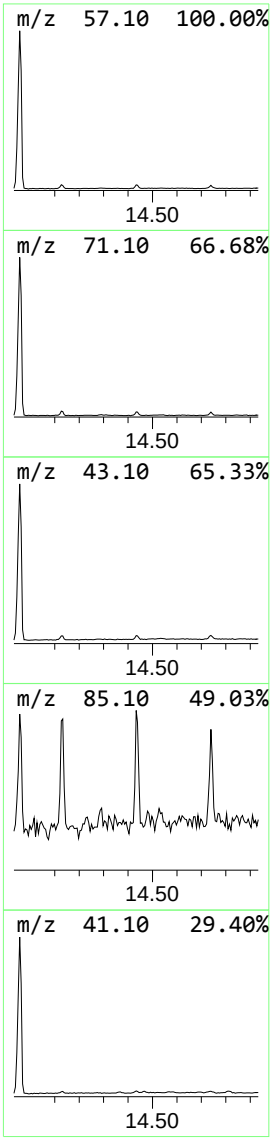
****

Peak Number 8 Behenyl chloride Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.433	2.74 ng	58690	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenyl chloride	344	C22H45Cl	042217-03-8	64
2	Heptacosane	380	C27H56	000593-49-7	60
3	Nonadecane	268	C19H40	000629-92-5	49
4	Tetracosane	338	C24H50	000646-31-1	47
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	46





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Instrument :
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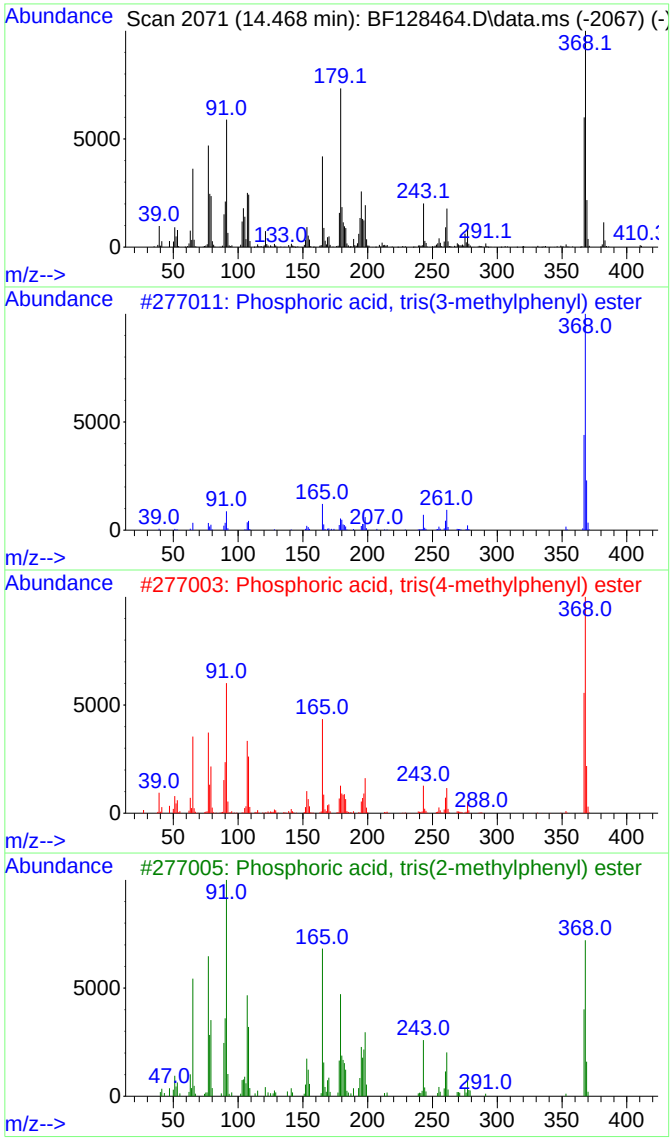
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

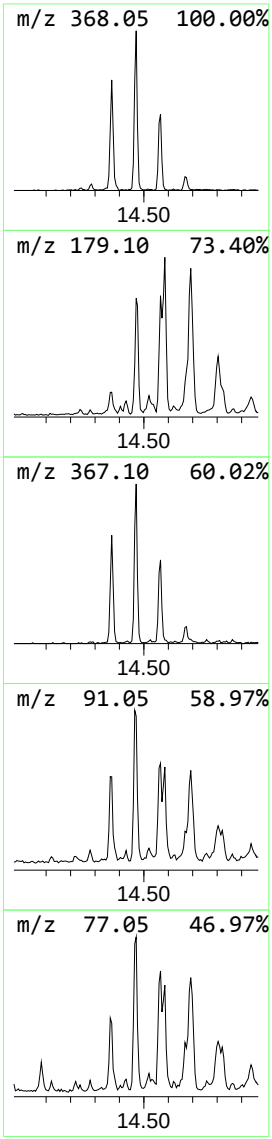
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Phosphoric acid, tris(3-met... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.468	24.36 ng	522647	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phosphoric acid, tris(3-methylph...	368	C21H21O4P	000563-04-2	99
2	Phosphoric acid, tris(4-methylph...	368	C21H21O4P	000078-32-0	99
3	Phosphoric acid, tris(2-methylph...	368	C21H21O4P	000078-30-8	87
4	4,4'-(4,4'-Biphenylylenedioxy)di...	368	C24H20N2O2	013080-85-8	18
5	1H-imidazole-4-carboxylic acid, ...	368	C24H20N2O2	1000398-59-0	18





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Data File : BF128464.D
Acq On : 25 May 2022 17:23
Operator : CG\JU
Sample : N2896-16
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P039-SS001-2430-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.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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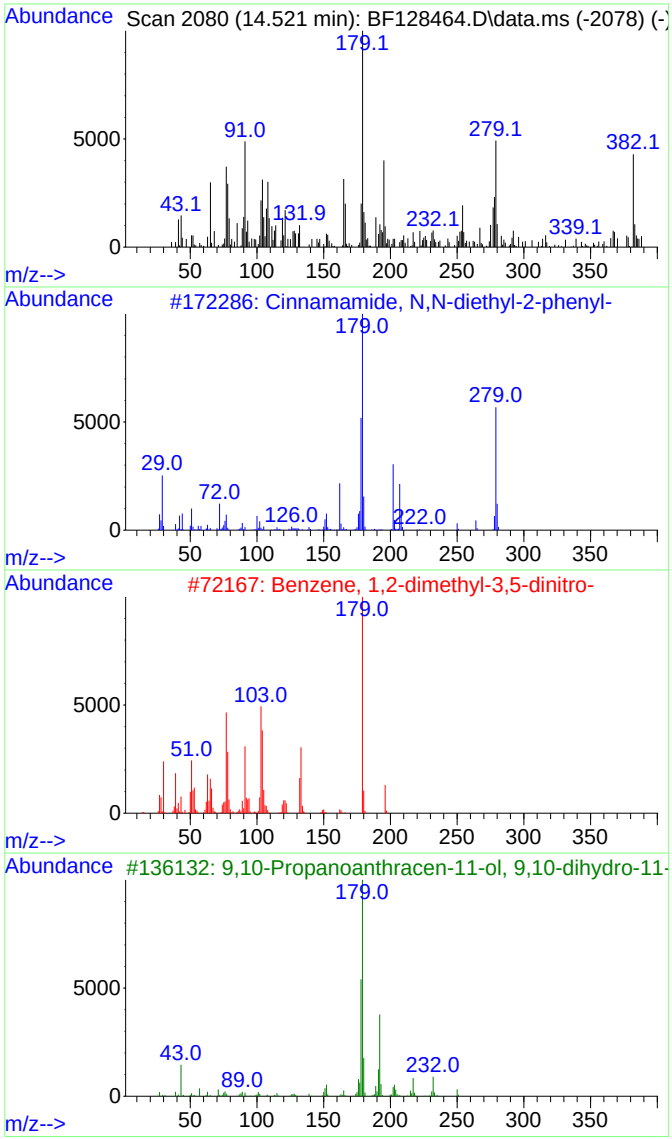
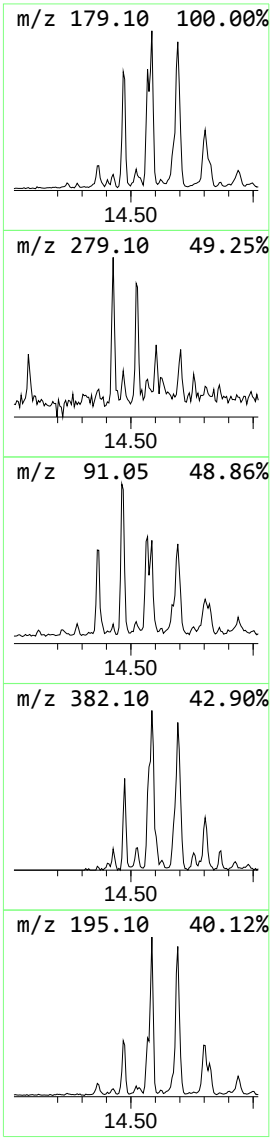
Peak Number 10 unknown14.521 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.521	3.76 ng	80658	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamamide, N,N-diethyl-2-phenyl-	279	C19H21NO	1000152-60-9	43
2	Benzene, 1,2-dimethyl-3,5-dinitro-	196	C8H8N2O4	000616-69-3	20
3	9,10-Propanoanthracen-11-ol, 9,1...	250	C18H18O	110163-81-0	18
4	Benzo[h]quinoline	179	C13H9N	000230-27-3	18
5	Phenanthridine	179	C13H9N	000229-87-8	18





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Acq On : 25 May 2022 17:23
Operator : CG\JU
Sample : N2896-16
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P039-SS001-2430-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.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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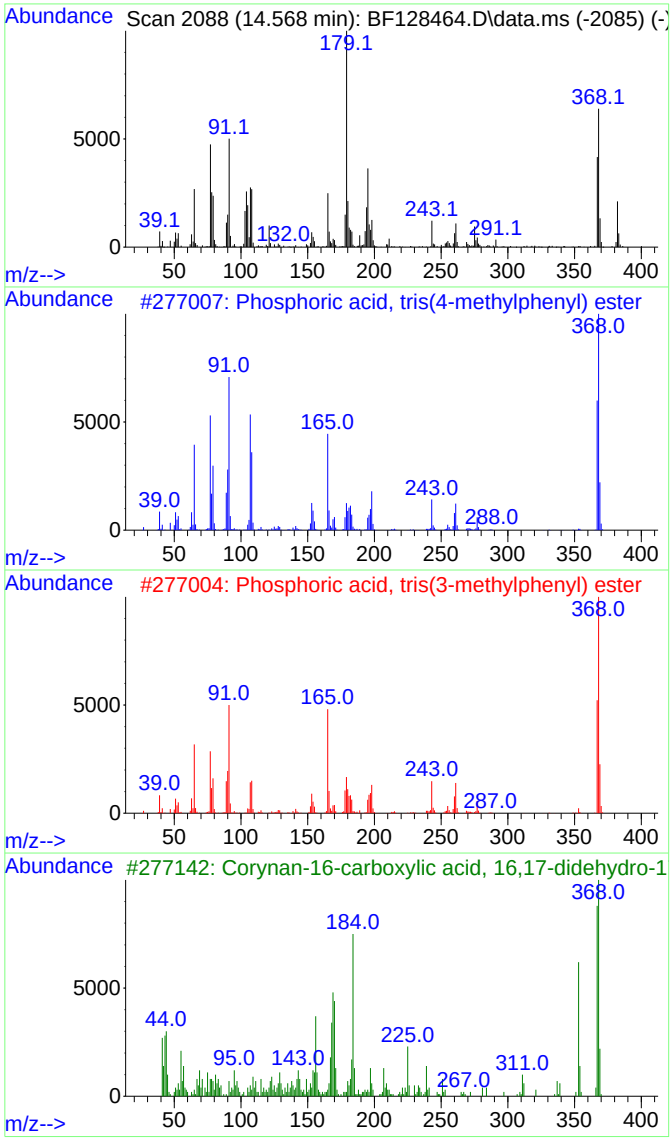
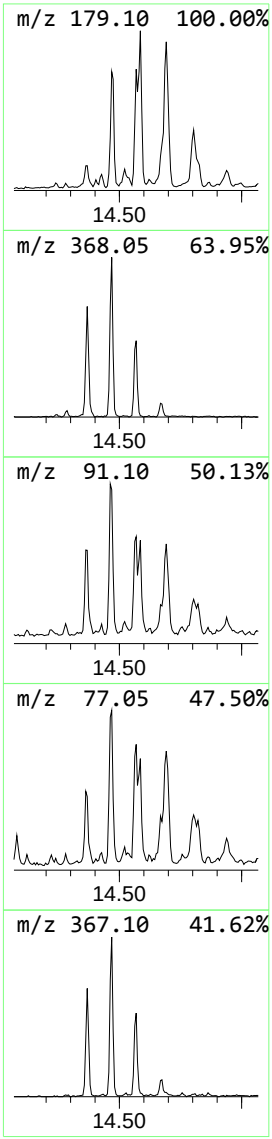
Peak Number 11 Phosphoric acid, tris(4-met... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.568	16.69 ng	358115	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phosphoric acid, tris(4-methylph...	368	C21H21O4P	000078-32-0	97
2	Phosphoric acid, tris(3-methylph...	368	C21H21O4P	000563-04-2	94
3	Corynan-16-carboxylic acid, 16,1...	368	C22H28N2O3	050439-68-4	25
4	5-Chloro-2-ethyl-3-methyl-1H-pyr...	194	C10H11ClN2	1000486-81-3	25
5	4,6-Dinitro-1,3-dimethyl-benzene	196	C8H8N2O4	000616-72-8	22





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Data File : BF128464.D
Acq On : 25 May 2022 17:23
Operator : CG\JU
Sample : N2896-16
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P039-SS001-2430-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.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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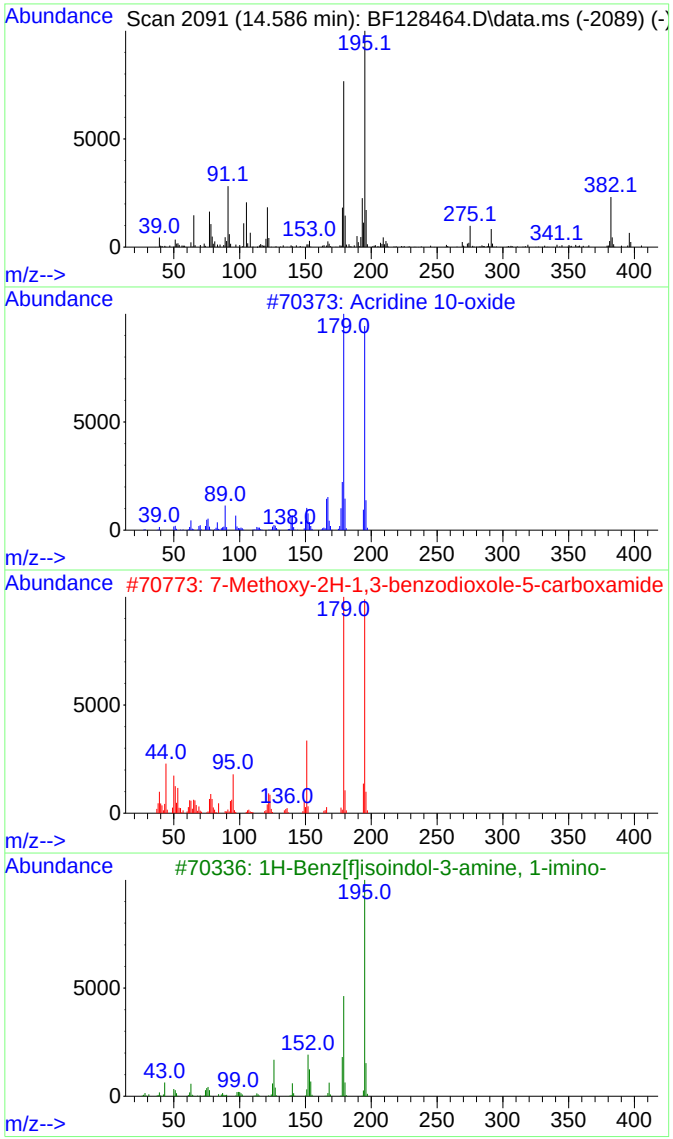
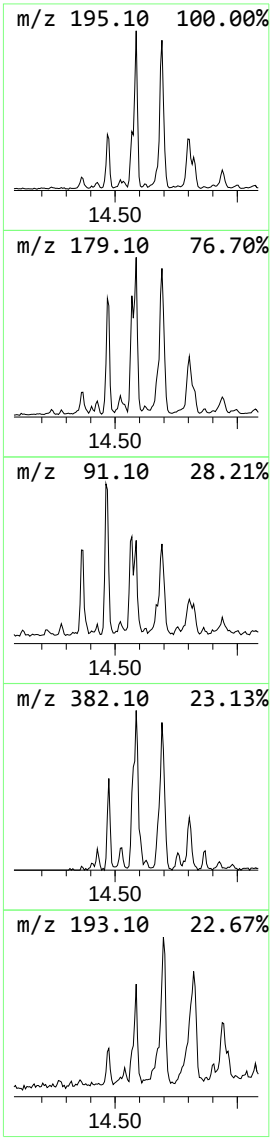
Peak Number 12 Acridine 10-oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.586	14.31 ng	307089	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acridine 10-oxide	195	C13H9NO	010399-73-2	58
2	7-Methoxy-2H-1,3-benzodioxole-5-...	195	C9H9NO4	114426-25-4	53
3	1H-Benz[f]isoindol-3-amine, 1-im...	195	C12H9N3	065558-69-2	46
4	Fluorenone oxime	195	C13H9NO	002157-52-0	35
5	2,5-Dimethyl-1,3-dinitrobenzene	196	C8H8N2O4	1010487-00-2	30





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Data File : BF128464.D
Acq On : 25 May 2022 17:23
Operator : CG\JU
Sample : N2896-16
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P039-SS001-2430-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.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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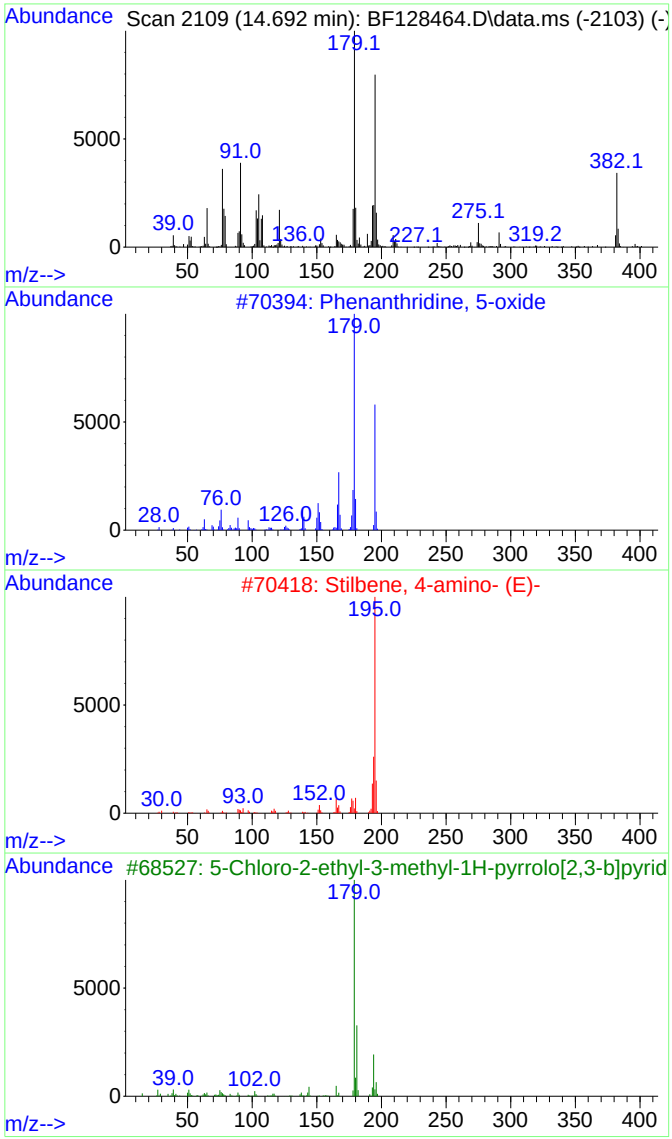
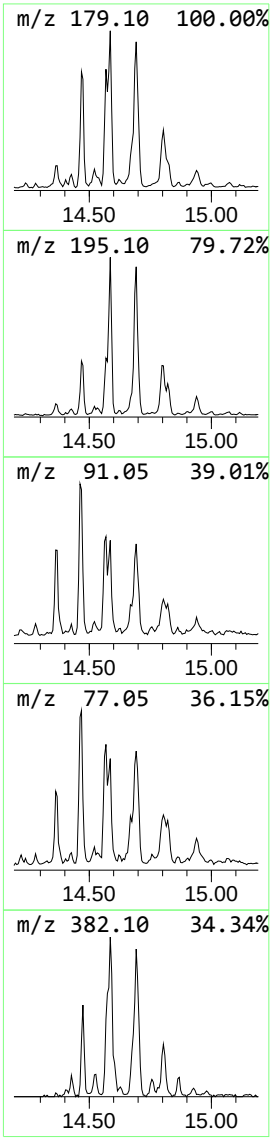
Peak Number 13 Phenanthridine, 5-oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.692	24.04 ng	515766	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthridine, 5-oxide	195	C13H9NO	014548-01-7	50
2	Stilbene, 4-amino- (E)-	195	C14H13N	004309-66-4	41
3	5-Chloro-2-ethyl-3-methyl-1H-pyr...	194	C10H11ClN2	1000486-81-3	35
4	[1,2,4]Triazolo[1,5-a]pyridine, ...	195	C12H9N3	000779-24-8	30
5	Terephthalic acid, ethyl nonyl e...	320	C19H28O4	1000323-74-3	27





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Data File : BF128464.D
Acq On : 25 May 2022 17:23
Operator : CG\JU
Sample : N2896-16
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P039-SS001-2430-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.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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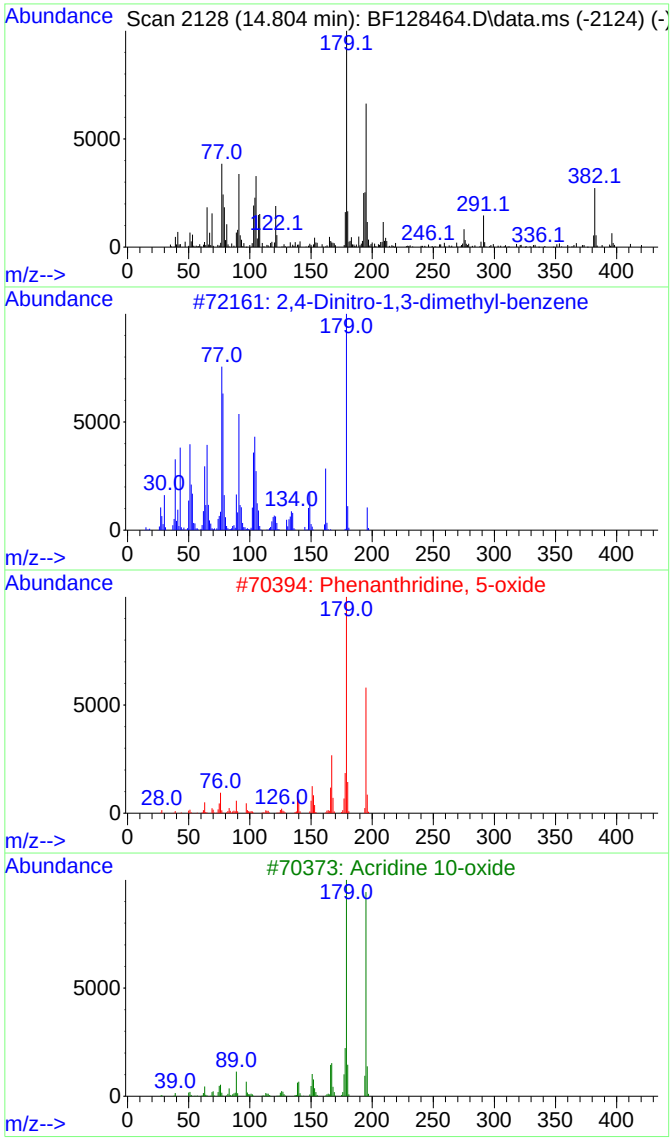
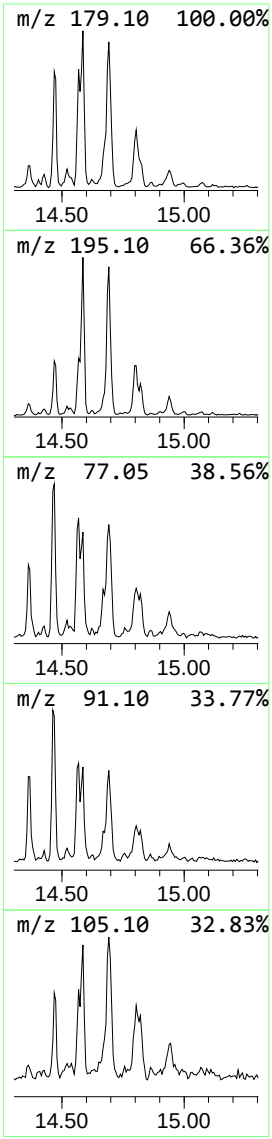
Peak Number 14 unknown14.804 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.804	23.39 ng	354210	Perylene-d12	15.462

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Dinitro-1,3-dimethyl-benzene	196	C8H8N2O4	000603-02-1	49
2	Phenanthridine, 5-oxide	195	C13H9NO	014548-01-7	35
3	Acridine 10-oxide	195	C13H9NO	010399-73-2	35
4	5-Chloro-2-ethyl-3-methyl-1H-pyr...	194	C10H11ClN2	1000486-81-3	30
5	Semicarbazide, 4-phenethyl-3-thio-	195	C9H13N3S	021198-23-2	20





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052522\
Data File : BF128464.D
Acq On : 25 May 2022 17:23
Operator : CG\JU
Sample : N2896-16
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P039-SS001-2430-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.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
3-Heptanone, 5-...	6.116	20.0	ng	546497	1	6.810	547589	20.0
Heptadecane	13.486	2.0	ng	43669	5	13.992	429160	20.0
Phthalic acid, ...	13.798	5.3	ng	114078	5	13.992	429160	20.0
11H-Benzo[a]flu...	13.845	6.0	ng	128442	5	13.992	429160	20.0
Triphenylphosph...	14.080	2.3	ng	49939	5	13.992	429160	20.0
Heneicosane	14.127	2.6	ng	55234	5	13.992	429160	20.0
Phosphoric acid...	14.368	12.6	ng	269890	5	13.992	429160	20.0
Behenyl chloride	14.433	2.7	ng	58690	5	13.992	429160	20.0
Phosphoric acid...	14.468	24.4	ng	522647	5	13.992	429160	20.0
unknown14.521	14.521	3.8	ng	80658	5	13.992	429160	20.0
Phosphoric acid...	14.568	16.7	ng	358115	5	13.992	429160	20.0
Acridine 10-oxide	14.586	14.3	ng	307089	5	13.992	429160	20.0
Phenanthridine,...	14.692	24.0	ng	515766	5	13.992	429160	20.0
unknown14.804	14.804	23.4	ng	354210	6	15.462	302911	20.0