LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052922\
Data File : BF128583.D
Acq On : 29 May 2022 20:59
Operator : CG\JU
Sample : N2951-21
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P036-SS001-0612-02

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-BF052622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128583.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.051	466	470	477	rVB	27553	35515	1.57%	0.184%
2	5.451	533	538	541	rBV	2108685	1898462	83.66%	9.857%
3	6.463	706	710	713	rBV	1899084	1789483	78.86%	9.291%
4	6.581	727	730	733	rBV	29151	24000	1.06%	0.125%
5	6.839	770	774	777	rBV	746173	573848	25.29%	2.980%
6	7.239	837	842	851	rVB	62322	63775	2.81%	0.331%
7	7.398	865	869	872	rBV	1396299	1166371	51.40%	6.056%
8	8.122	988	992	995	rBV	823075	645830	28.46%	3.353%
9	9.198	1170	1175	1178	rBV	2415023	1954449	86.13%	10.148%
10	9.874	1287	1290	1294	rBV	805626	728021	32.08%	3.780%
11	10.663	1420	1424	1428	rBV	1558164	1427005	62.88%	7.409%
12	10.692	1428	1429	1434	rVB2	42294	37227	1.64%	0.193%
13	10.998	1475	1481	1484	rBV	34206	31483	1.39%	0.163%
14	11.139	1502	1505	1508	rBB	192600	149969	6.61%	0.779%
15	11.257	1519	1525	1529	rVB6	16890	24775	1.09%	0.129%
16	11.363	1540	1543	1547	rBV	956883	810052	35.70%	4.206%
17	11.892	1629	1633	1637	rBV	449692	448365	19.76%	2.328%
18	11.927	1637	1639	1642	rVB	47906	43071	1.90%	0.224%
19	12.210	1682	1687	1692	rVB3	29899	39065	1.72%	0.203%
20	12.451	1723	1728	1733	rBV6	26542	56869	2.51%	0.295%
21	12.680	1763	1767	1777	rBV2	184085	234155	10.32%	1.216%
22	12.951	1809	1813	1817	rBV	2460496	2269297	100.00%	11.783%
23	13.186	1850	1853	1857	rBV3	23167	33002	1.45%	0.171%
24	13.227	1857	1860	1864	rVB	60981	56187	2.48%	0.292%
25	13.427	1892	1894	1898	rVB3	26747	26871	1.18%	0.140%
26	13.815	1955	1960	1965	rBV	684695	577015	25.43%	2.996%
27	13.880	1965	1971	1981	rBV2	207353	486436	21.44%	2.526%
28	14.004	1987	1992	1996	rBV	833767	786940	34.68%	4.086%
29	14.104	2005	2009	2013	rBV	366219	360917	15.90%	1.874%
30	14.145	2013	2016	2019	rVV	491676	441813	19.47%	2.294%
31	14.180	2019	2022	2025	rVV	720147	673202	29.67%	3.495%
32	14.209	2025	2027	2029	rVV	248972	206486	9.10%	1.072%
33	14.233	2029	2031	2035	rVB	260348	229370	10.11%	1.191%
34	14.480	2071	2073	2077	rVB	48661	40434	1.78%	0.210%
35	14.527	2078	2081	2088	rVV	129430	130649	5.76%	0.678%
36	14.768	2119	2122	2124	rBV	102989	99930	4.40%	0.519%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052922\
Data File : BF128583.D
Acq On : 29 May 2022 20:59
Operator : CG\JU
Sample : N2951-21
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P036-SS001-0612-02

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-BF052622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.133	2181	2184	2187	rVB	62982	70324	3.10%	0.365%
38	15.468	2237	2241	2246	rBV	403742	509961	22.47%	2.648%
39	15.515	2246	2249	2254	rVB3	59196	78977	3.48%	0.410%

Sum of corrected areas: 19259601

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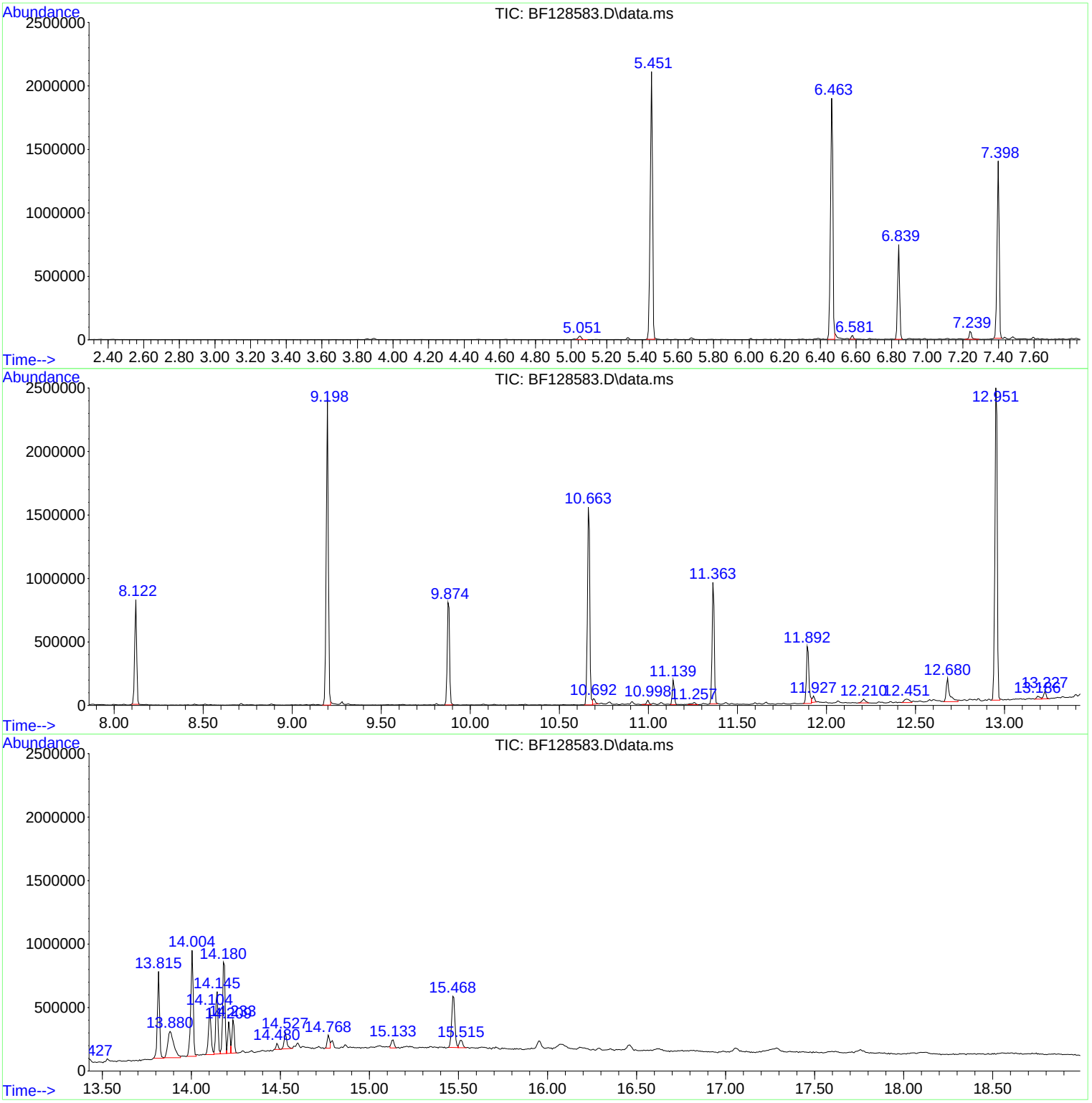
BNA_F
ClientSampleId :
P036-SS001-0612-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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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Operator : CG\JU
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Misc :
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Instrument :
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P036-SS001-0612-02

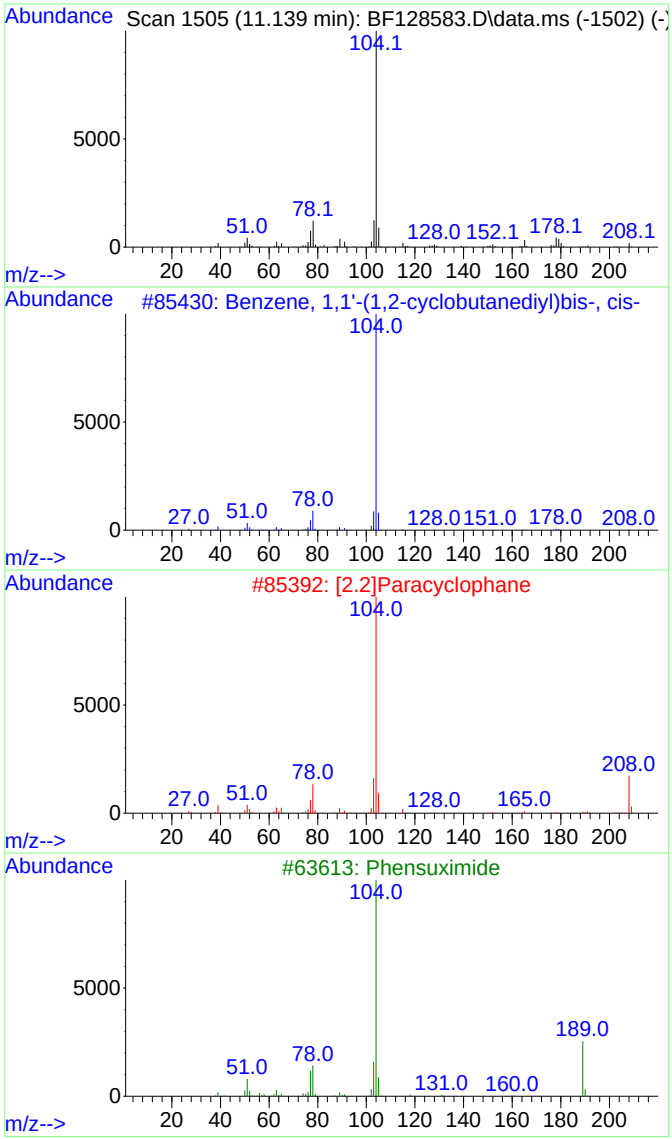
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

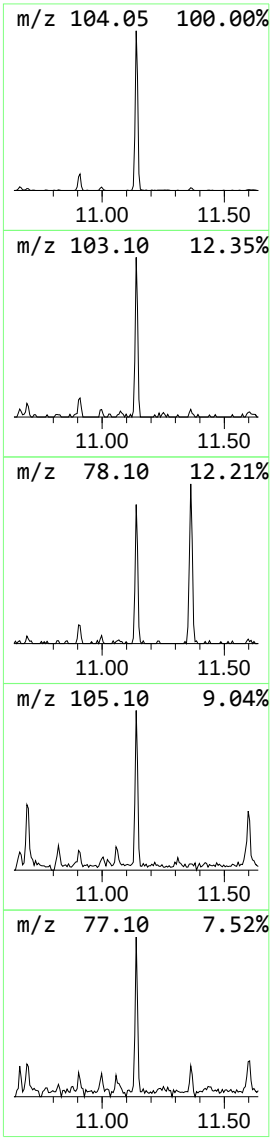
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Benzene, 1,1'-(1,2-cyclobut... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.139	3.70 ng	149969	Phenanthrene-d10	11.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-(1,2-cyclobutanedi...	208	C16H16	007694-30-6	91
2	[2.2]Paracyclophane	208	C16H16	001633-22-3	87
3	Phensuximide	189	C11H11NO2	000086-34-0	83
4	1,3,7-Octatrien-5-yne	104	C8H8	016607-77-5	58
5	Carphedon, N-(trifluoroacetyl)	314	C14H13F3N2O3	1000445-42-6	56





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

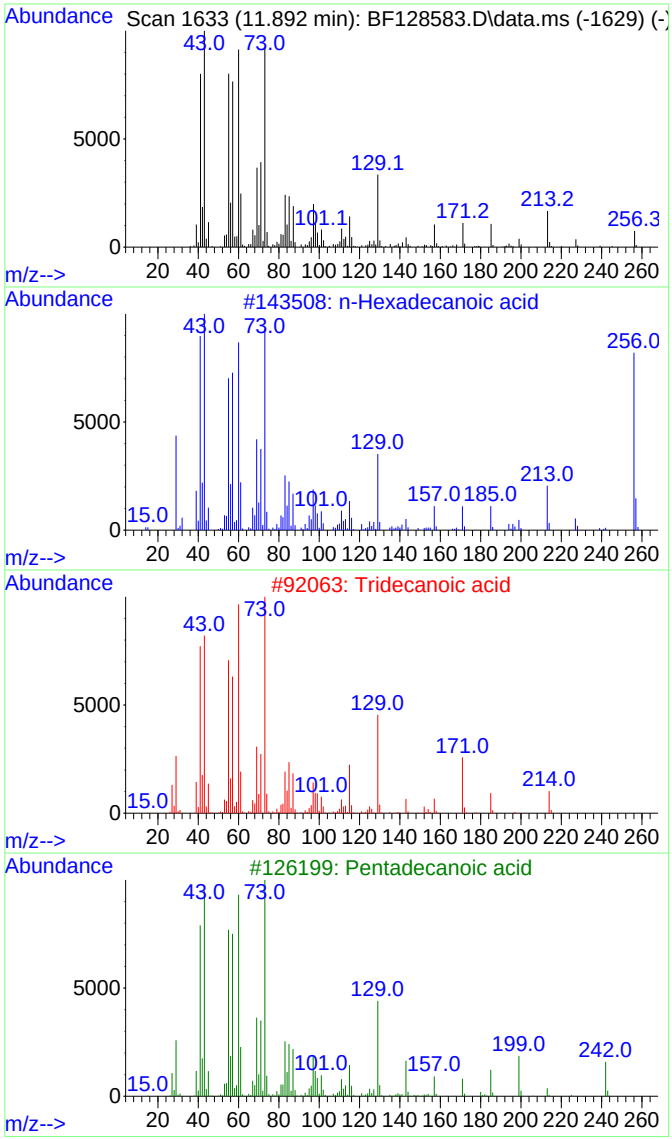
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

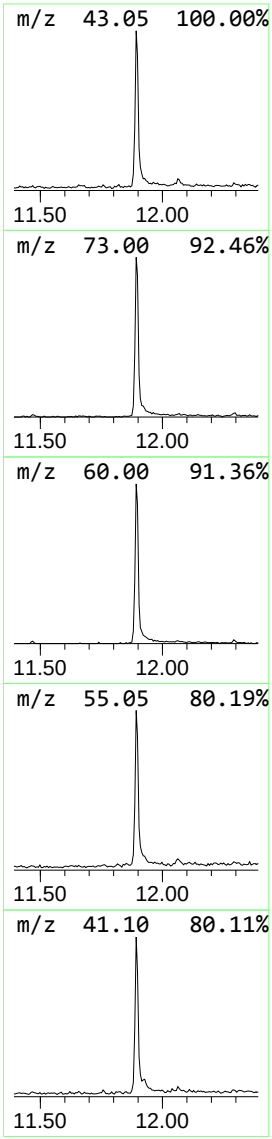
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	11.07 ng	448365	Phenanthrene-d10	11.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052922\
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Operator : CG\JU
Sample : N2951-21
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P036-SS001-0612-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

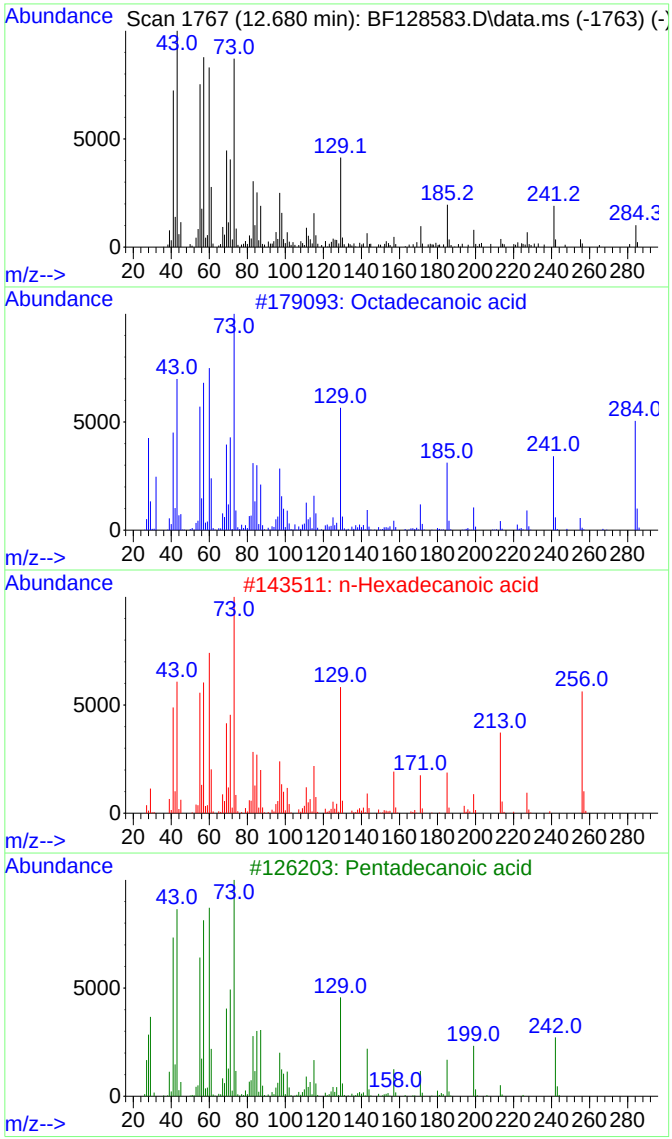
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

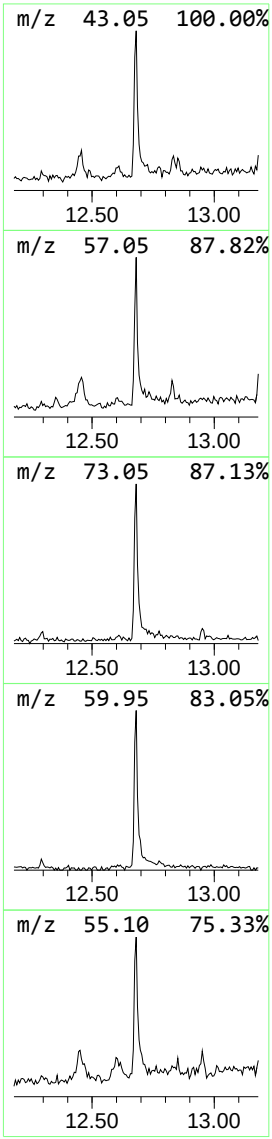
****

Peak Number 3 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.680	5.78 ng	234155	Phenanthrene-d10	11.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052922\
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Acq On : 29 May 2022 20:59
Operator : CG\JU
Sample : N2951-21
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P036-SS001-0612-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

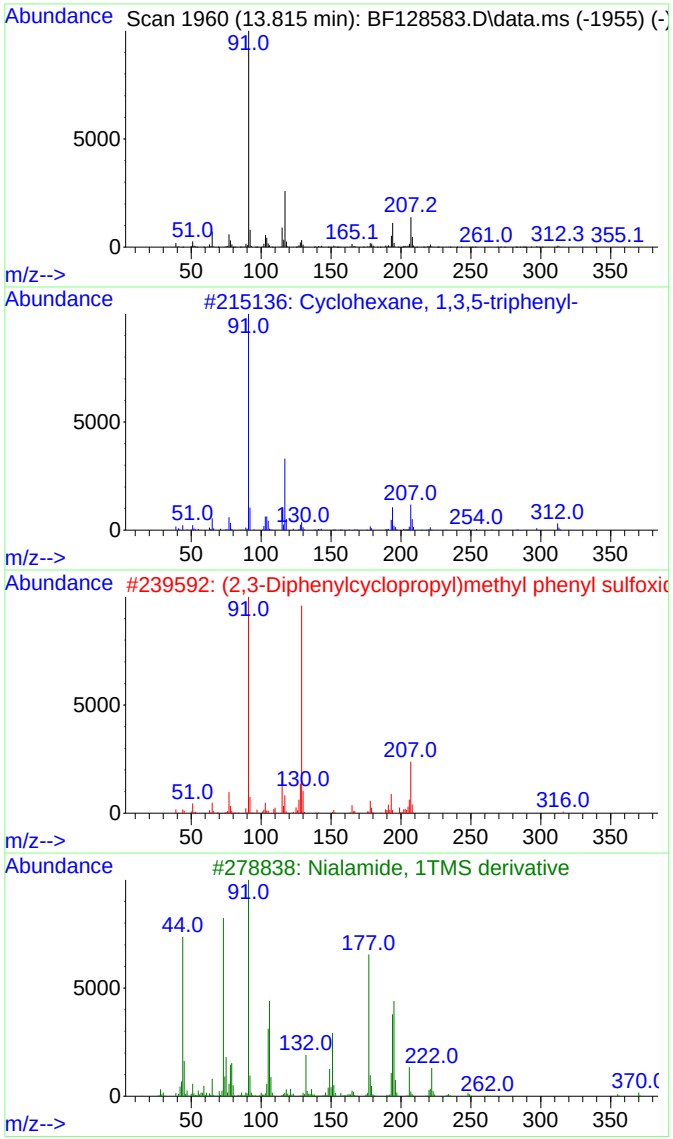
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

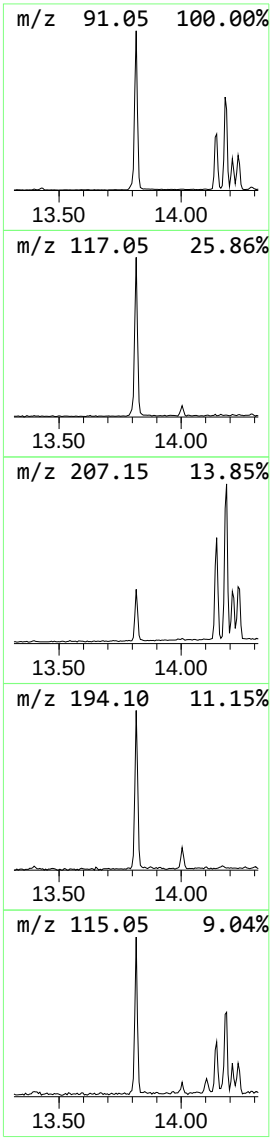
****

Peak Number 4 Cyclohexane, 1,3,5-triphenyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.815	14.66 ng	577015	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,3,5-triphenyl-	312	C24H24	028336-57-4	72
2	(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	32
3	Nialamide, 1TMS derivative	370	C19H26N4O2Si	1000485-79-3	22
4	Carbonic acid, monoamide, N-benz...	207	C12H17NO2	1000451-48-5	12
5	Phenol, 2-(phenylmethoxy)-	200	C13H12O2	006272-38-4	11





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052922\
Data File : BF128583.D
Acq On : 29 May 2022 20:59
Operator : CG\JU
Sample : N2951-21
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P036-SS001-0612-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

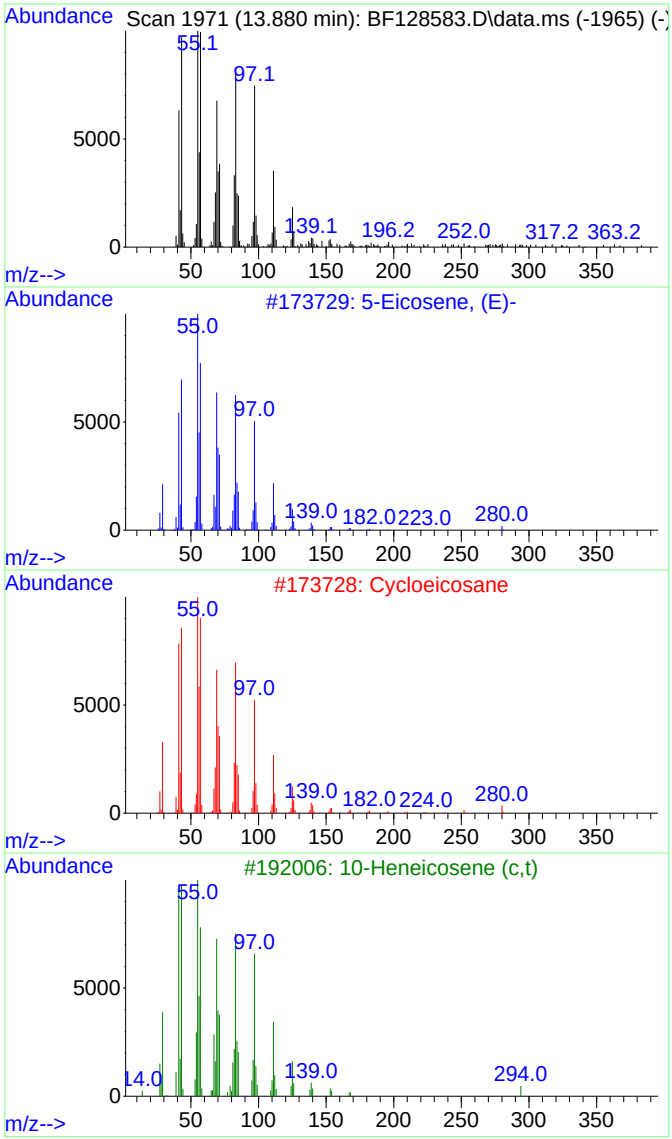
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

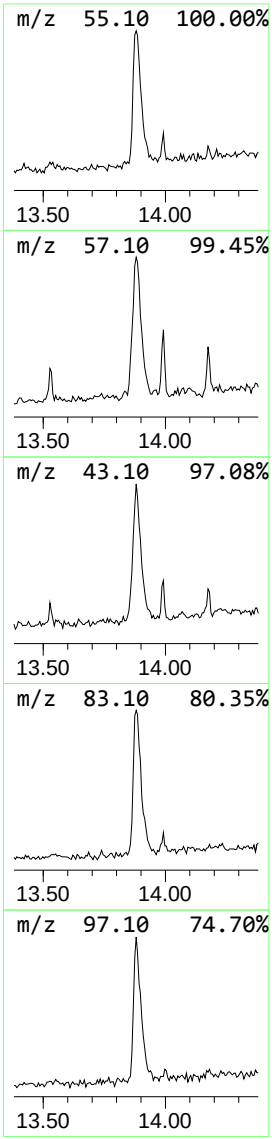
****

Peak Number 5 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	12.36 ng	486436	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2	Cycloeicosane	280	C20H40	000296-56-0	95
3	10-Heneicosene (c,t)	294	C21H42	095008-11-0	95
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	93





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Instrument :
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ClientSampleId :
P036-SS001-0612-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

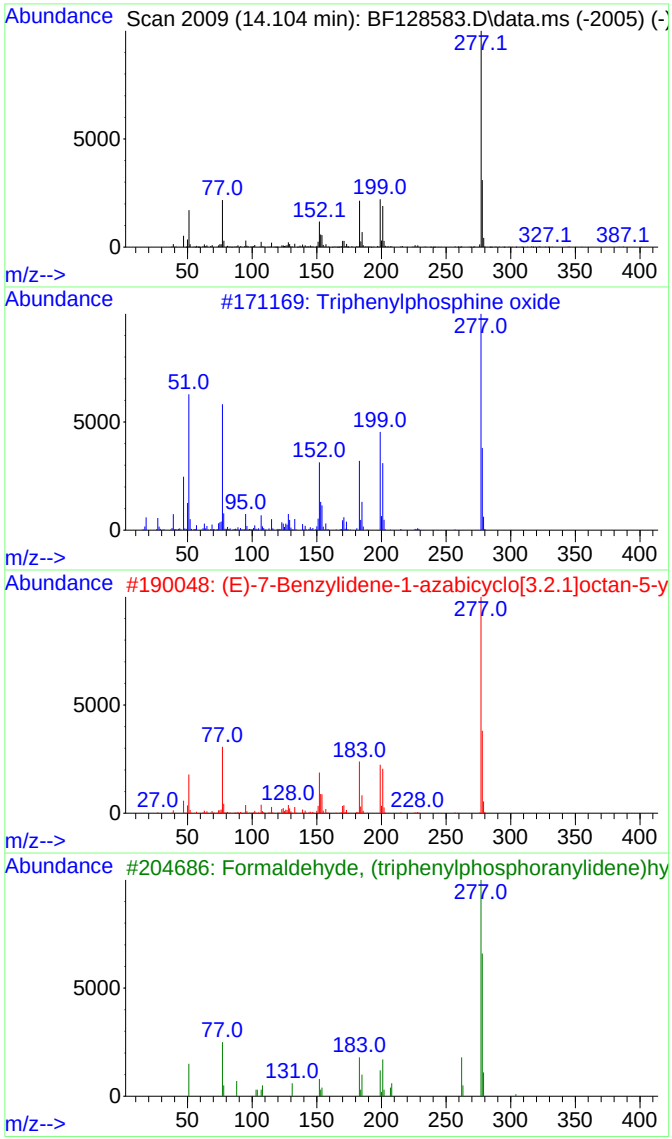
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

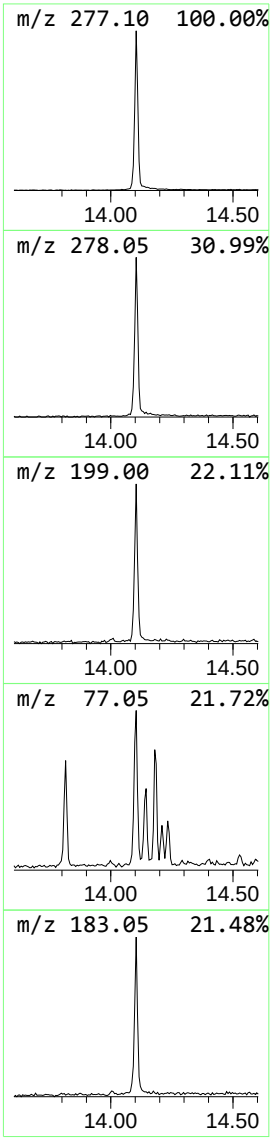
****

Peak Number 6 Triphenylphosphine oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.104	9.17 ng	360917	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	70
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	38
5	3-(3,4-Dichlorophenyl)-2-thioxo-...	277	C9H5Cl2NOS2	017046-34-3	25





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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

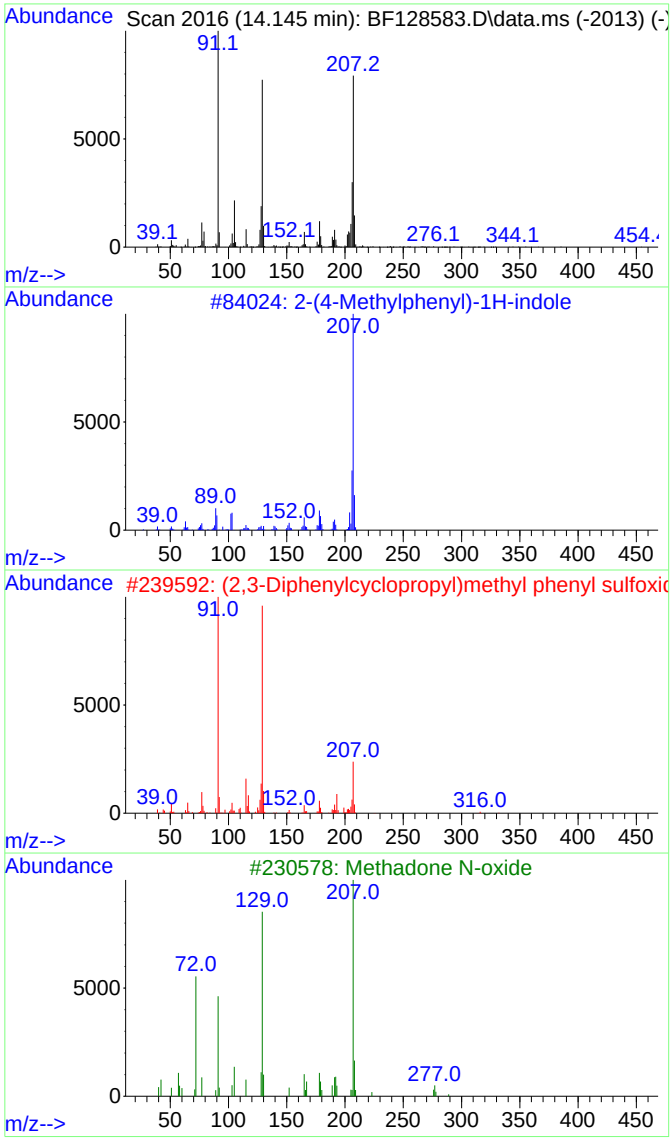
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

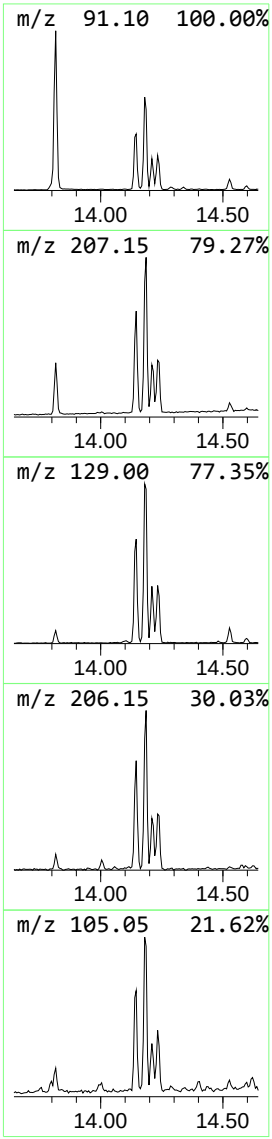
****

Peak Number 7 2-(4-Methylphenyl)-1H-indole Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.145	11.23 ng	441813	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(4-Methylphenyl)-1H-indole	207	C15H13N	055577-25-8	86
2	(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	72
3	Methadone N-oxide	325	C21H27NO2	1000120-80-7	47
4	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	46
5	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	46





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Data File : BF128583.D
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ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P036-SS001-0612-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

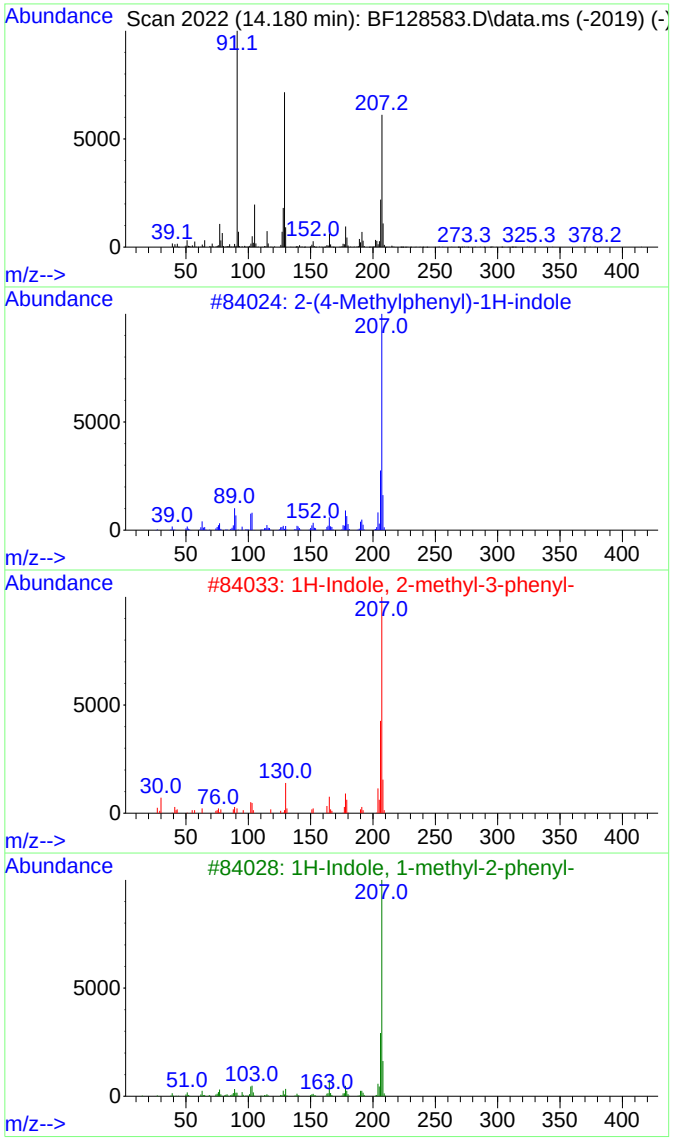
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

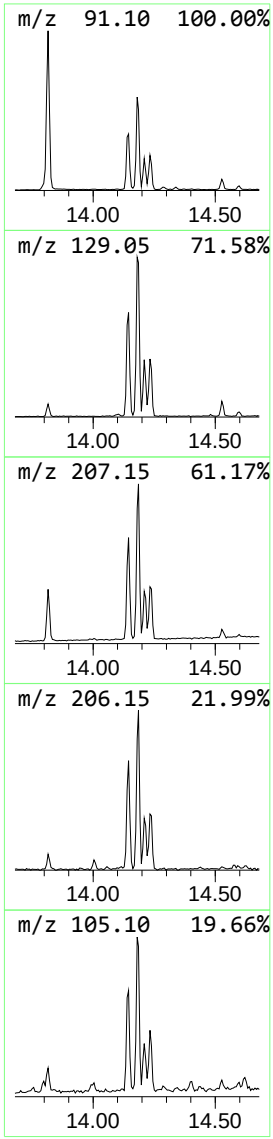
****

Peak Number 8 unknown14.180 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.180	17.11 ng	673202	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(4-Methylphenyl)-1H-indole	207	C15H13N	055577-25-8	46
2	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	45
3	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	42
4	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	27
5	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	25





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ClientSampleId :
P036-SS001-0612-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

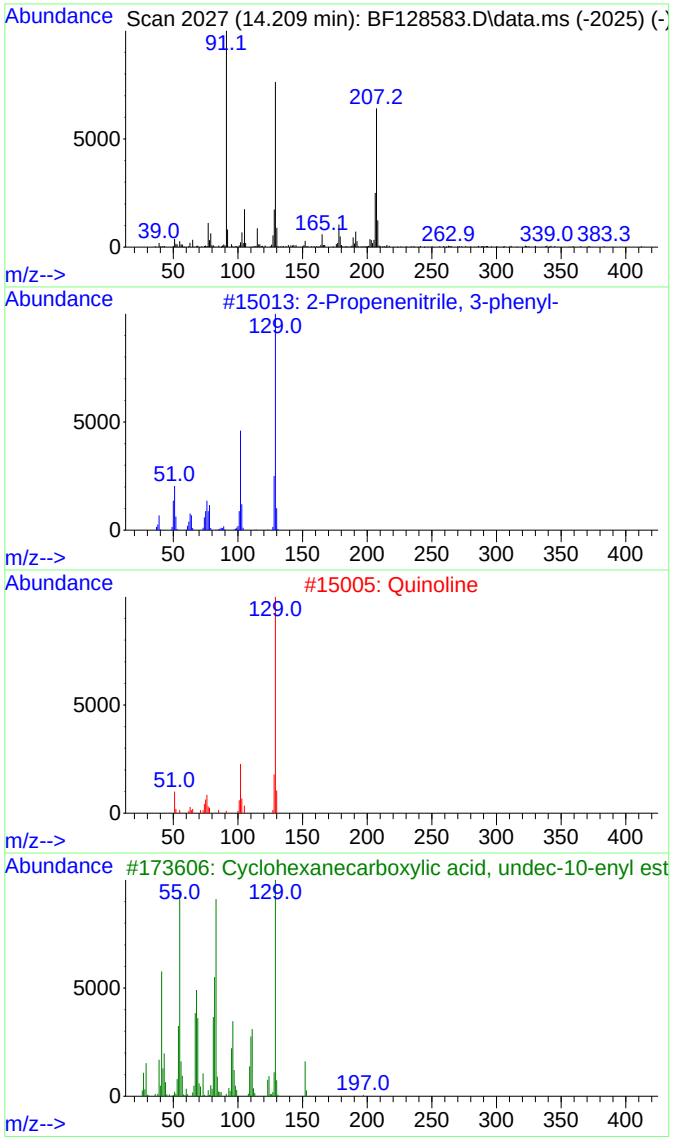
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

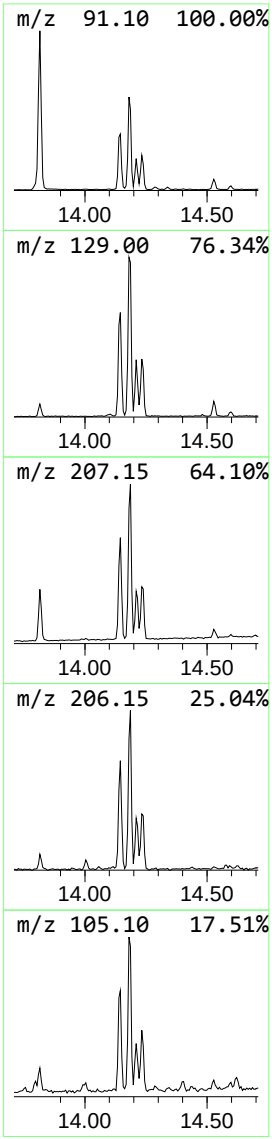
****

Peak Number 9 unknown14.210 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.210	5.25 ng	206486	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenenitrile, 3-phenyl-	129	C9H7N	004360-47-8	35
2	Quinoline	129	C9H7N	000091-22-5	35
3	Cyclohexanecarboxylic acid, unde...	280	C18H32O2	1000279-53-9	35
4	Isoquinoline	129	C9H7N	000119-65-3	35
5	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052922\
Data File : BF128583.D
Acq On : 29 May 2022 20:59
Operator : CG\JU
Sample : N2951-21
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P036-SS001-0612-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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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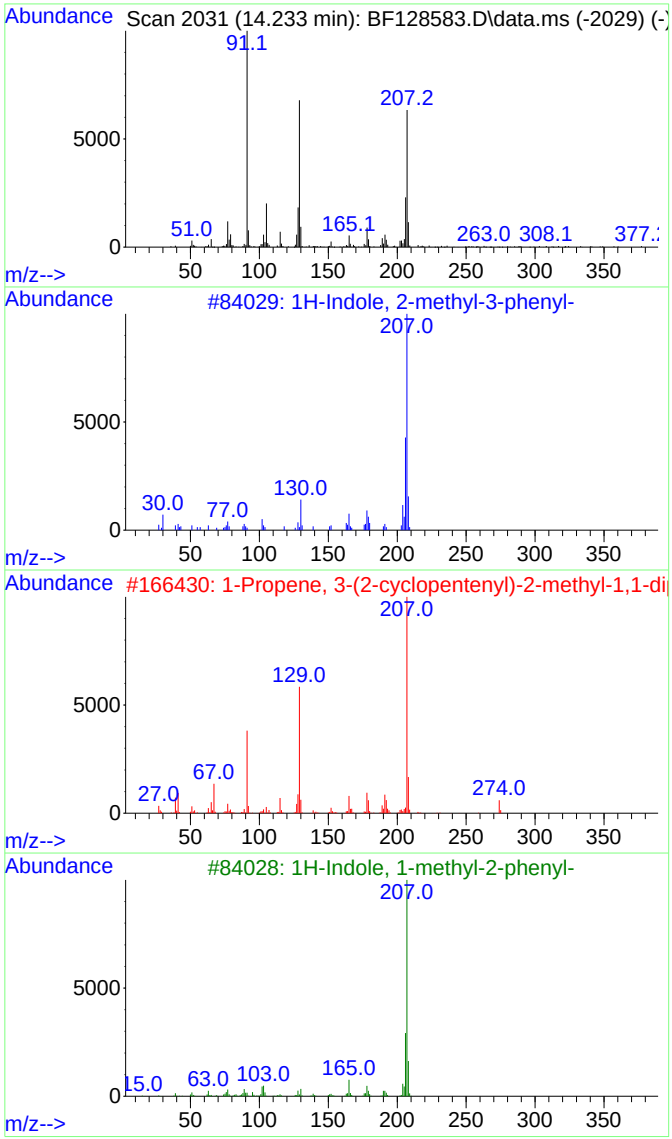
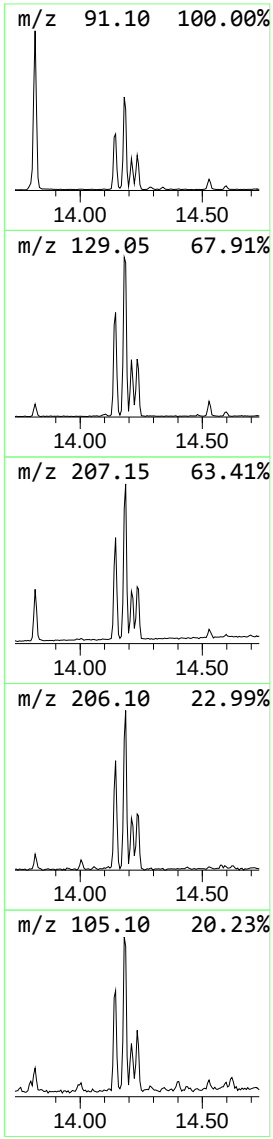
Peak Number 10 1H-Indole, 2-methyl-3-phenyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.233	5.83 ng	229370	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	50
2	1-Propene, 3-(2-cyclopentenyl)-2...	274	C21H22	1010154-23-3	43
3	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	42
4	2-(4-Methylphenyl)-1H-indole	207	C15H13N	055577-25-8	41
5	1-benzylindole	207	C15H13N	1000334-31-3	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052922\
Data File : BF128583.D
Acq On : 29 May 2022 20:59
Operator : CG\JU
Sample : N2951-21
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P036-SS001-0612-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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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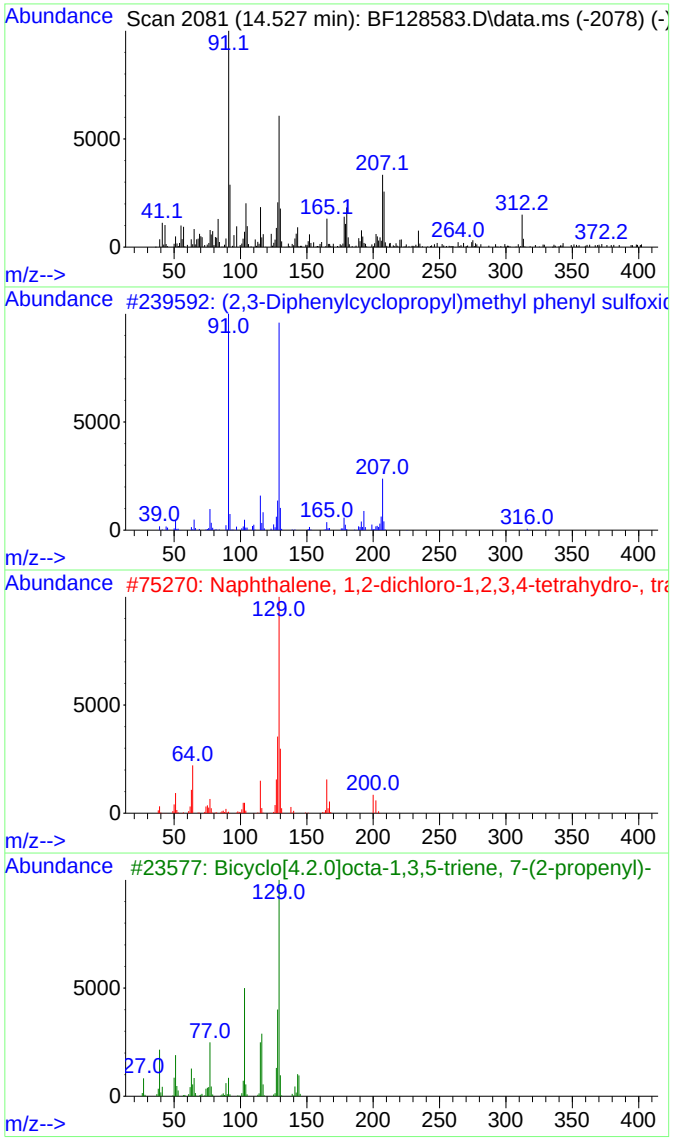
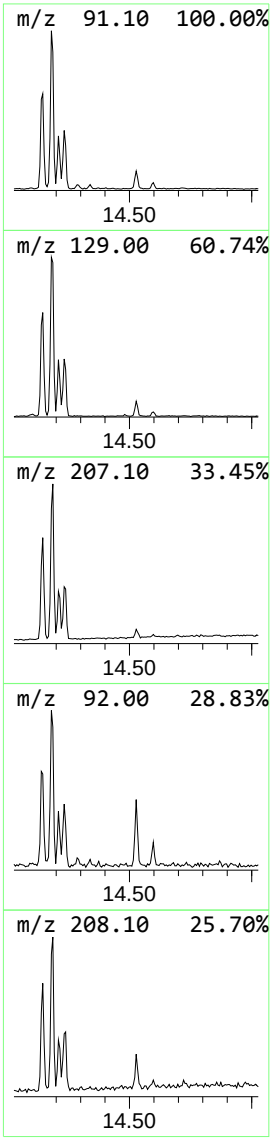
Peak Number 11 unknown14.527 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.527	3.32 ng	130649	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	35
2	Naphthalene, 1,2-dichloro-1,2,3,...	200	C10H10Cl2	031448-63-2	22
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	144	C11H12	071721-26-1	22
4	Benzonitrile, 4-ethenyl-	129	C9H7N	003435-51-6	22
5	(1-Ethylbuta-1,3-dienyl)benzene	158	C12H14	1000210-05-6	22





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Acq On : 29 May 2022 20:59
Operator : CG\JU
Sample : N2951-21
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P036-SS001-0612-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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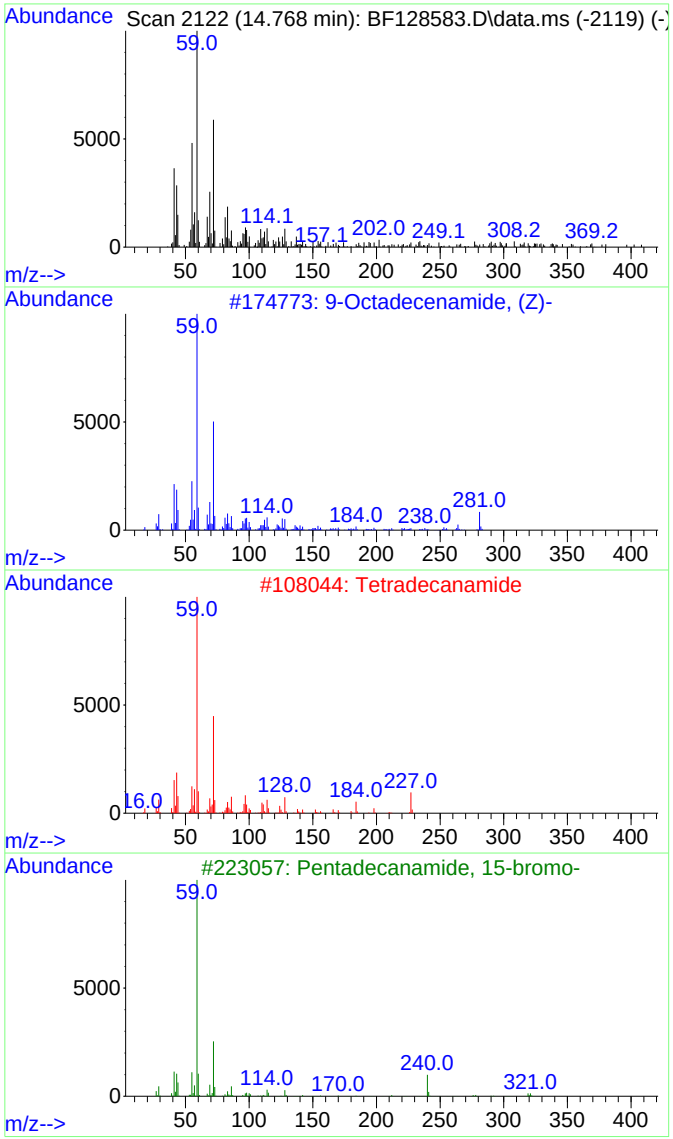
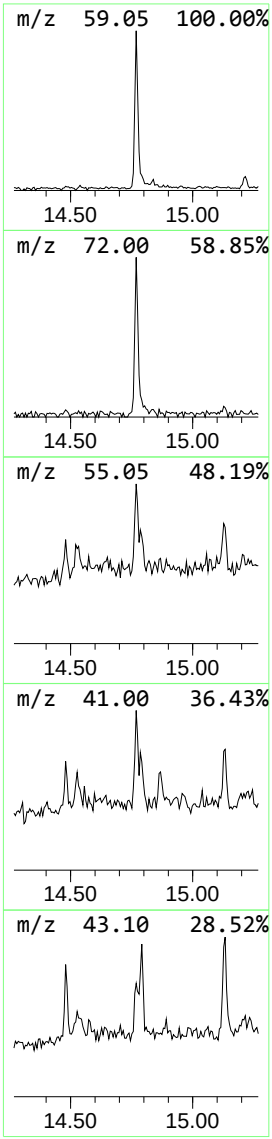
Peak Number 12 9-Octadecenamide, (Z)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.768	3.92 ng	99930	Perylene-d12	15.474

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2	Tetradecanamide	227	C14H29NO	000638-58-4	64
3	Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	58
4	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	58
5	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	52





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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P036-SS001-0612-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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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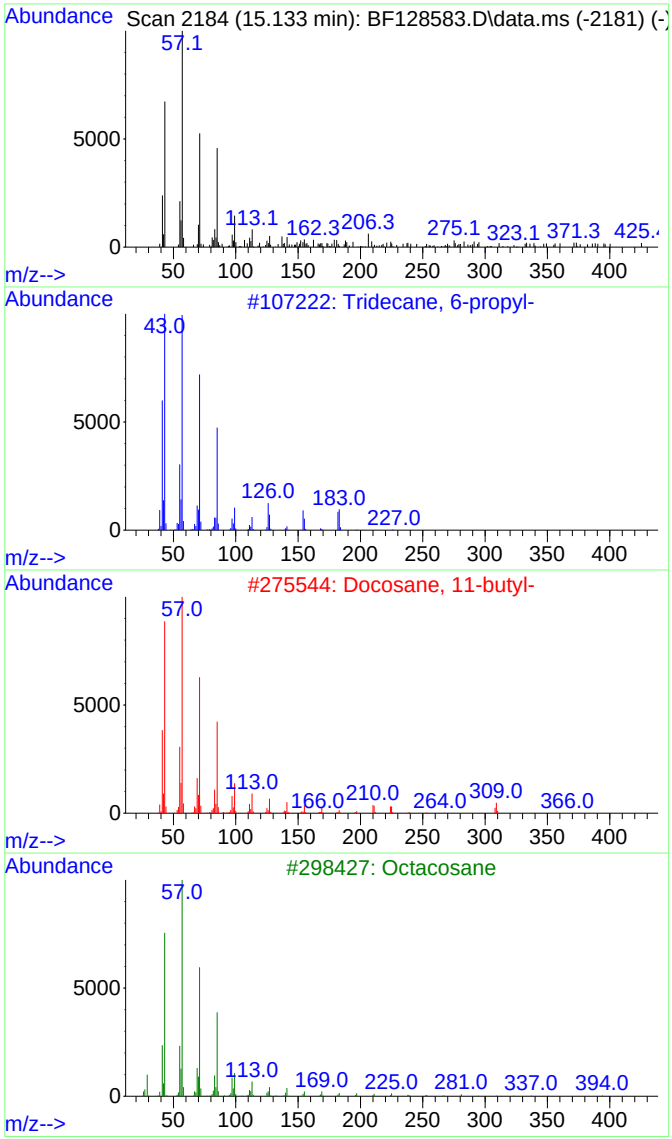
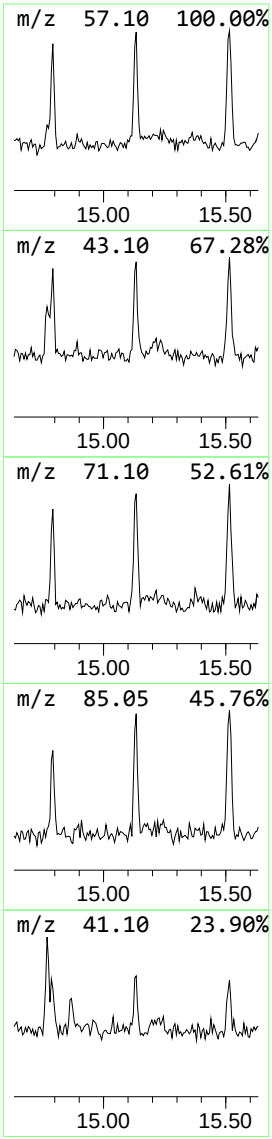
Peak Number 13 Tridecane, 6-propyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.133	2.76 ng	70324	Perylene-d12	15.474

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 6-propyl-	226	C16H34	055045-10-8	91
2	Docosane, 11-butyl-	366	C26H54	013475-76-8	83
3	Octacosane	394	C28H58	000630-02-4	83
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83
5	Heptadecane	240	C17H36	000629-78-7	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052922\
Data File : BF128583.D
Acq On : 29 May 2022 20:59
Operator : CG\JU
Sample : N2951-21
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P036-SS001-0612-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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
Benzene, 1,1'-(...	11.139	3.7	ng	149969	4	11.363	810052	20.0
n-Hexadecanoic ...	11.892	11.1	ng	448365	4	11.363	810052	20.0
Octadecanoic acid	12.680	5.8	ng	234155	4	11.363	810052	20.0
Cyclohexane, 1,...	13.815	14.7	ng	577015	5	14.004	786940	20.0
5-Eicosene, (E)-	13.880	12.4	ng	486436	5	14.004	786940	20.0
Triphenylphosph...	14.104	9.2	ng	360917	5	14.004	786940	20.0
2-(4-Methylphen...	14.145	11.2	ng	441813	5	14.004	786940	20.0
unknown14.180	14.180	17.1	ng	673202	5	14.004	786940	20.0
unknown14.210	14.210	5.3	ng	206486	5	14.004	786940	20.0
1H-Indole, 2-me...	14.233	5.8	ng	229370	5	14.004	786940	20.0
unknown14.527	14.527	3.3	ng	130649	5	14.004	786940	20.0
9-Octadecenamid...	14.768	3.9	ng	99930	6	15.474	509961	20.0
Tridecane, 6-pr...	15.133	2.8	ng	70324	6	15.474	509961	20.0