LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072225\
Data File : BF143207.D
Acq On : 23 Jul 2025 00:12
Operator : RC/JU
Sample : Q2649-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

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-BF071725.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF143207.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.304	12	19	27	rVB	492608	788929	39.82%	4.162%
2	5.198	505	511	519	rVB	151155	207421	10.47%	1.094%
3	5.604	574	580	585	rBV	1348991	1748836	88.26%	9.225%
4	6.598	743	749	754	rBV	1324537	1749097	88.27%	9.227%
5	6.969	807	812	817	rBV	520017	628576	31.72%	3.316%
6	7.522	900	906	911	rBV	936929	1169420	59.02%	6.169%
7	8.251	1024	1030	1037	rBV	606816	764756	38.60%	4.034%
8	9.322	1207	1212	1217	rBV	1637106	1981468	100.00%	10.452%
9	10.004	1323	1328	1333	rBV	593960	726049	36.64%	3.830%
10	10.410	1392	1397	1403	rBV	48237	71984	3.63%	0.380%
11	10.710	1443	1448	1457	rBV	168324	213790	10.79%	1.128%
12	10.792	1457	1462	1467	rBV	719060	893150	45.08%	4.711%
13	10.916	1478	1483	1490	rBV6	11003	20260	1.02%	0.107%
14	11.492	1576	1581	1590	rBV2	505107	777512	39.24%	4.101%
15	12.010	1662	1669	1681	rBV3	261601	497472	25.11%	2.624%
16	12.104	1681	1685	1693	rVB	42511	88485	4.47%	0.467%
17	12.304	1713	1719	1724	rVB3	23138	50049	2.53%	0.264%
18	12.545	1756	1760	1763	rBV2	20551	26110	1.32%	0.138%
19	12.627	1771	1774	1779	rVB2	20144	26935	1.36%	0.142%
20	12.704	1782	1787	1799	rBV	447622	861318	43.47%	4.544%
21	12.798	1799	1803	1811	rVB2	55164	100502	5.07%	0.530%
22	12.933	1820	1826	1832	rBV	329258	454118	22.92%	2.396%
23	13.074	1844	1850	1857	rVB	1316372	1672234	84.39%	8.821%
24	13.151	1859	1863	1870	rBV5	32123	58959	2.98%	0.311%
25	13.257	1875	1881	1885	rBV3	40520	85888	4.33%	0.453%
26	13.368	1896	1900	1906	rBV2	39515	58040	2.93%	0.306%
27	13.610	1938	1941	1944	rBV	27887	35574	1.80%	0.188%
28	13.762	1964	1967	1973	rVB	44896	60670	3.06%	0.320%
29	13.968	1998	2002	2009	rVB2	162596	253091	12.77%	1.335%
30	14.127	2021	2029	2040	rBV3	675185	1449484	73.15%	7.646%
31	15.192	2206	2210	2219	rVB	185048	415125	20.95%	2.190%
32	15.509	2261	2264	2270	rVB	107478	156582	7.90%	0.826%
33	15.574	2271	2275	2280	rVV	126463	197967	9.99%	1.044%
34	15.639	2282	2286	2300	rVB	371638	667031	33.66%	3.519%

Sum of corrected areas: 18956882

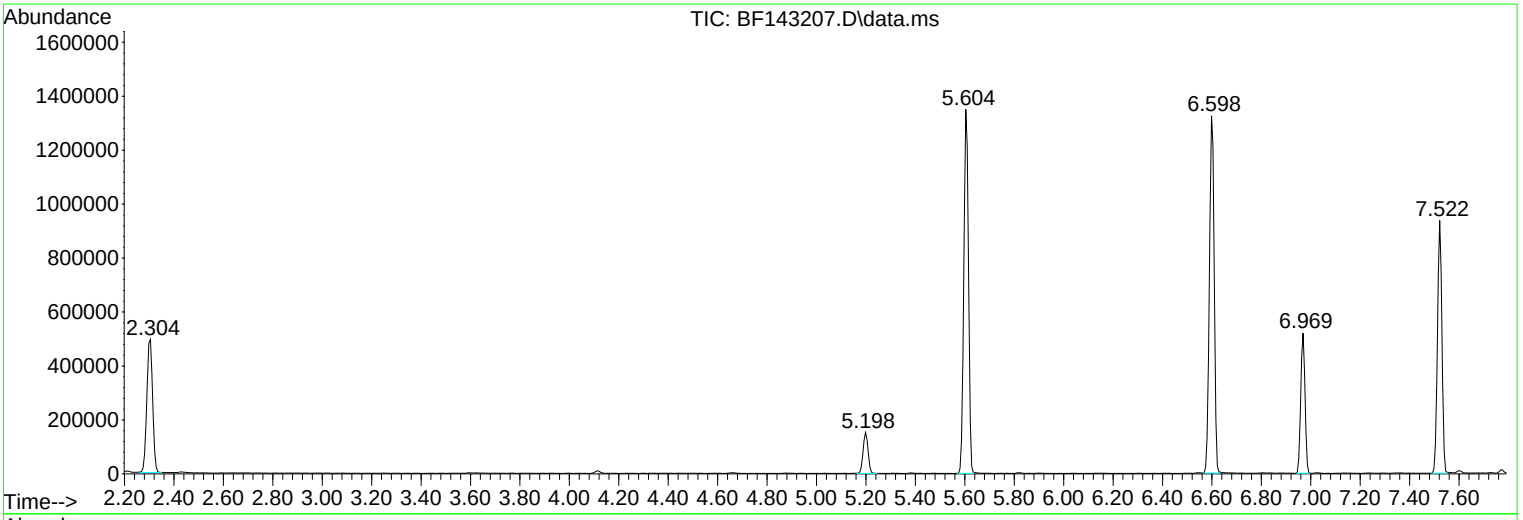
Instrument :
BNA_F
ClientSampleId :
WC-1

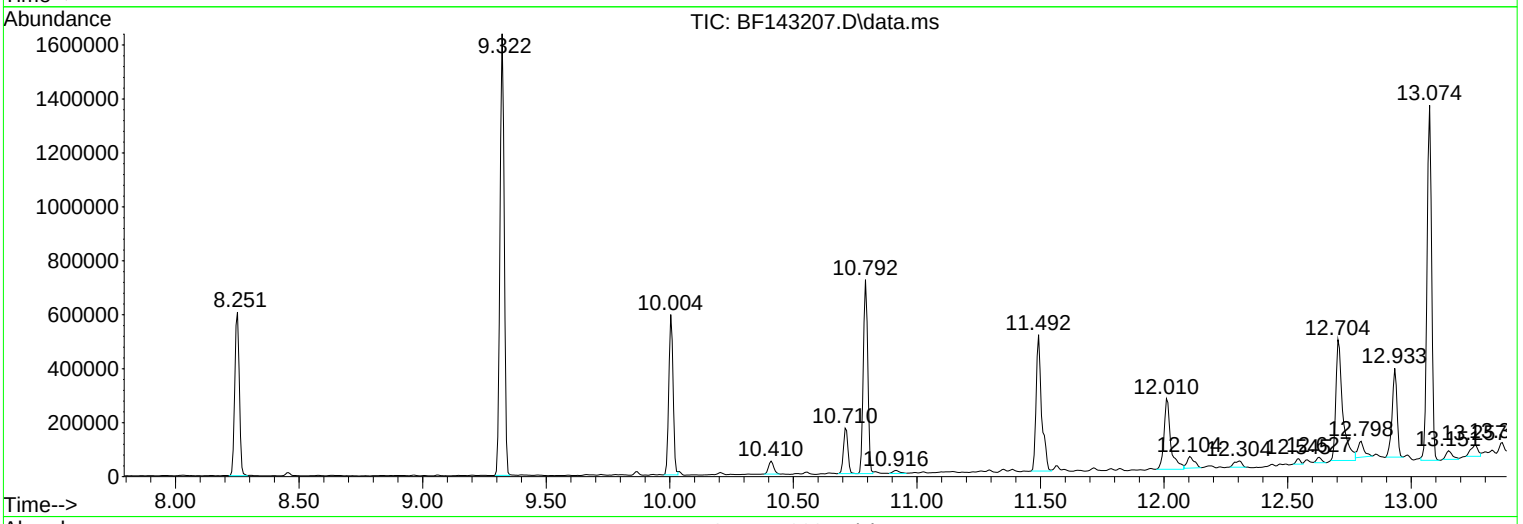
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072225\
Data File : BF143207.D
Acq On : 23 Jul 2025 00:12
Operator : RC/JU
Sample : Q2649-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

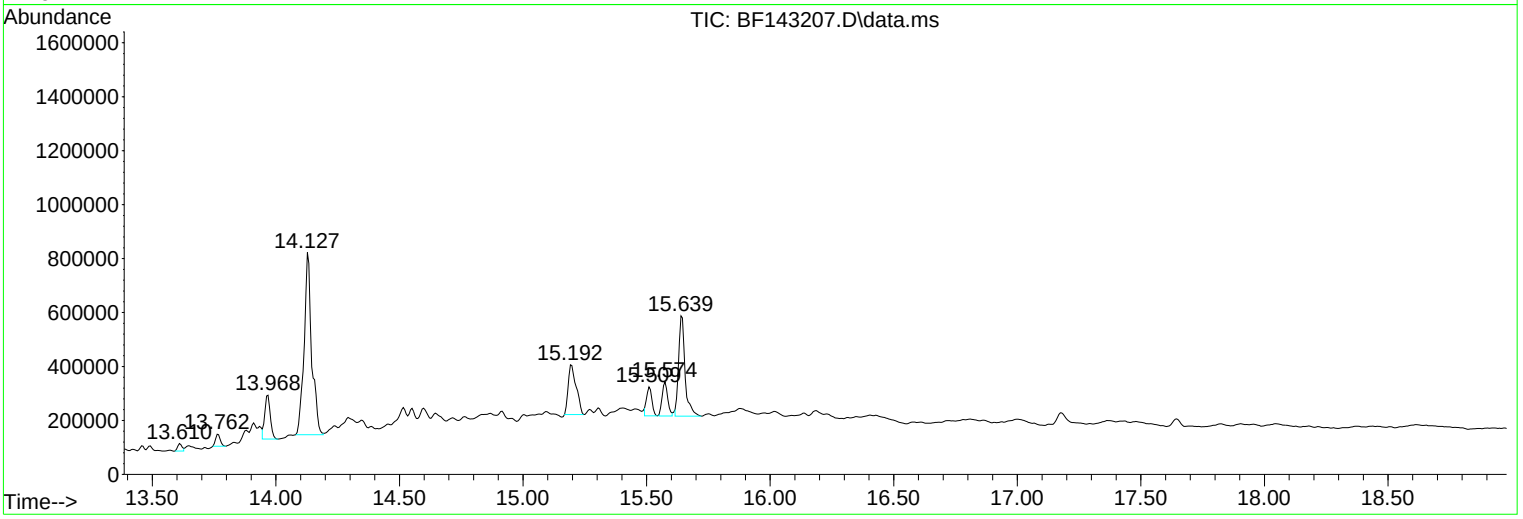
Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.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 : RC/JU
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

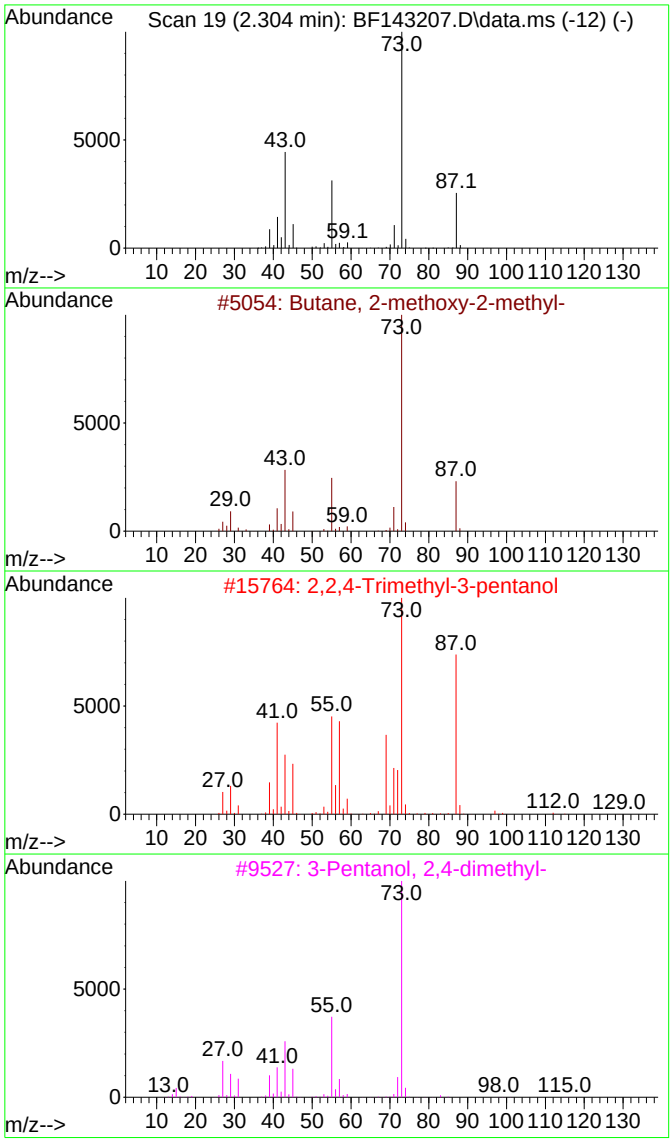
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

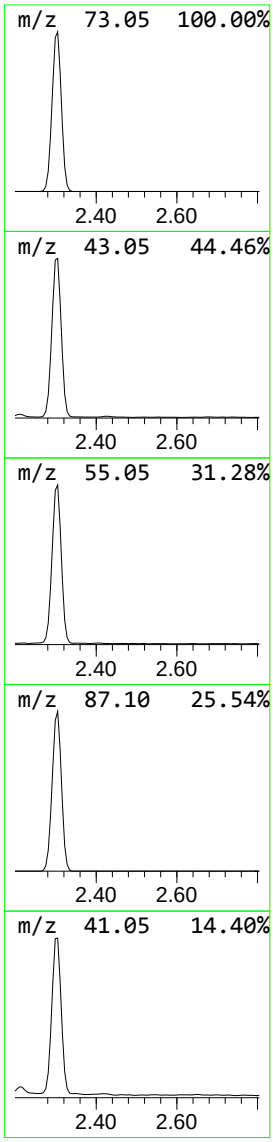
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.304	25.10 ng	788929	1,4-Dichlorobenzene-d4	6.969

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	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





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Operator : RC/JU
Sample : Q2649-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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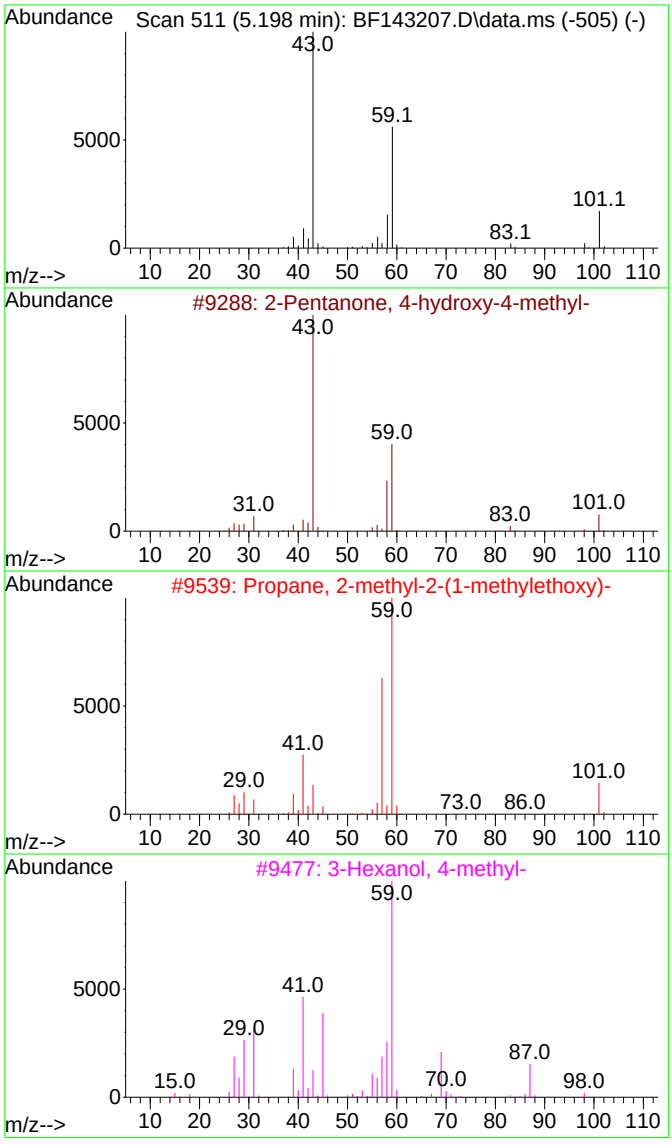
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

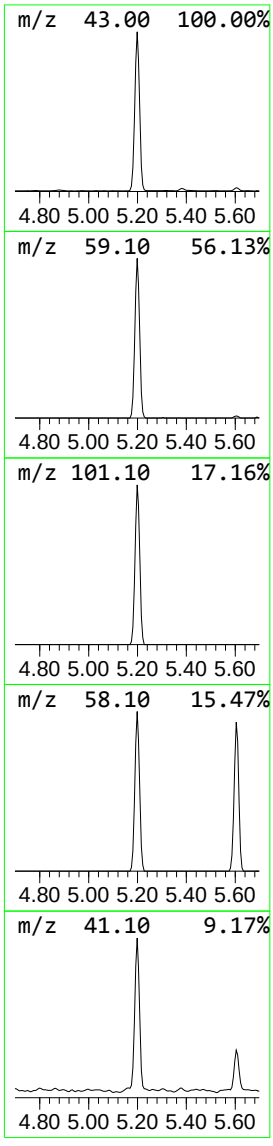
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.198	6.60 ng	207421	1,4-Dichlorobenzene-d4	6.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





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Acq On : 23 Jul 2025 00:12
Operator : RC/JU
Sample : Q2649-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.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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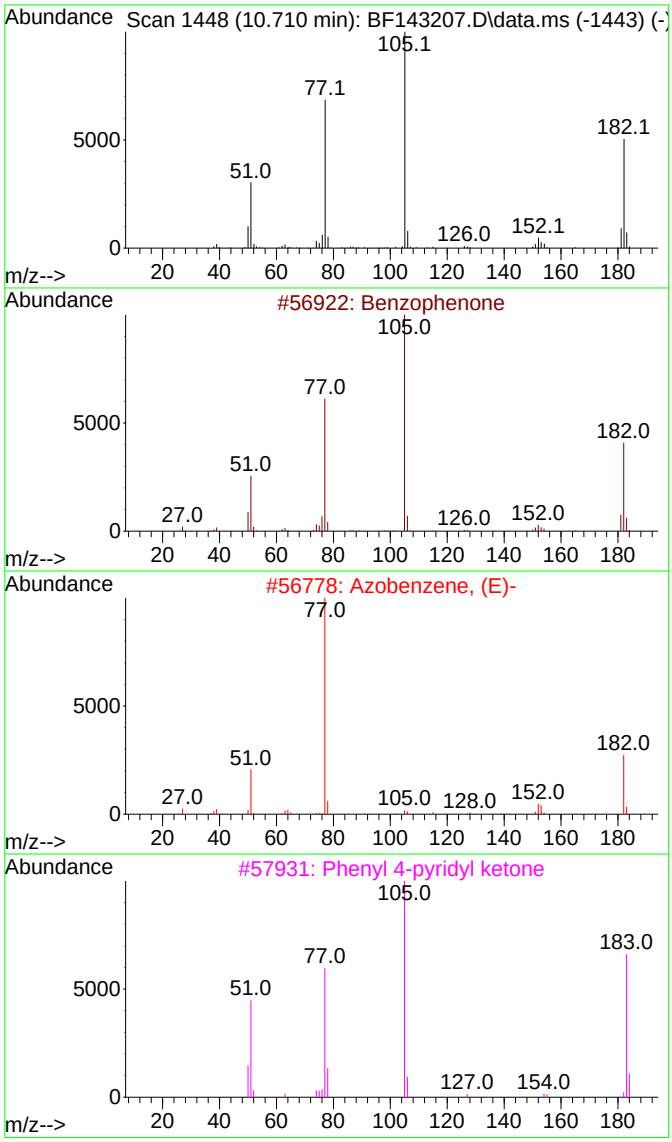
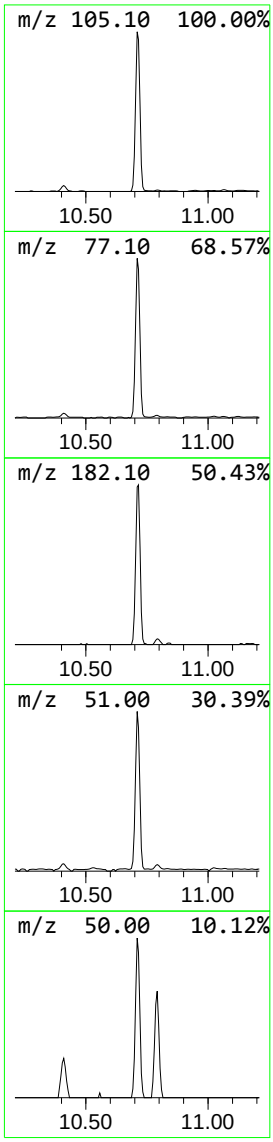
Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.710	5.89 ng	213790	Acenaphthene-d10	10.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene, (E)-	182	C12H10N2	017082-12-1	53
3	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
4	Benzoylformic acid	150	C8H6O3	000611-73-4	49
5	acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072225\
Data File : BF143207.D
Acq On : 23 Jul 2025 00:12
Operator : RC/JU
Sample : Q2649-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.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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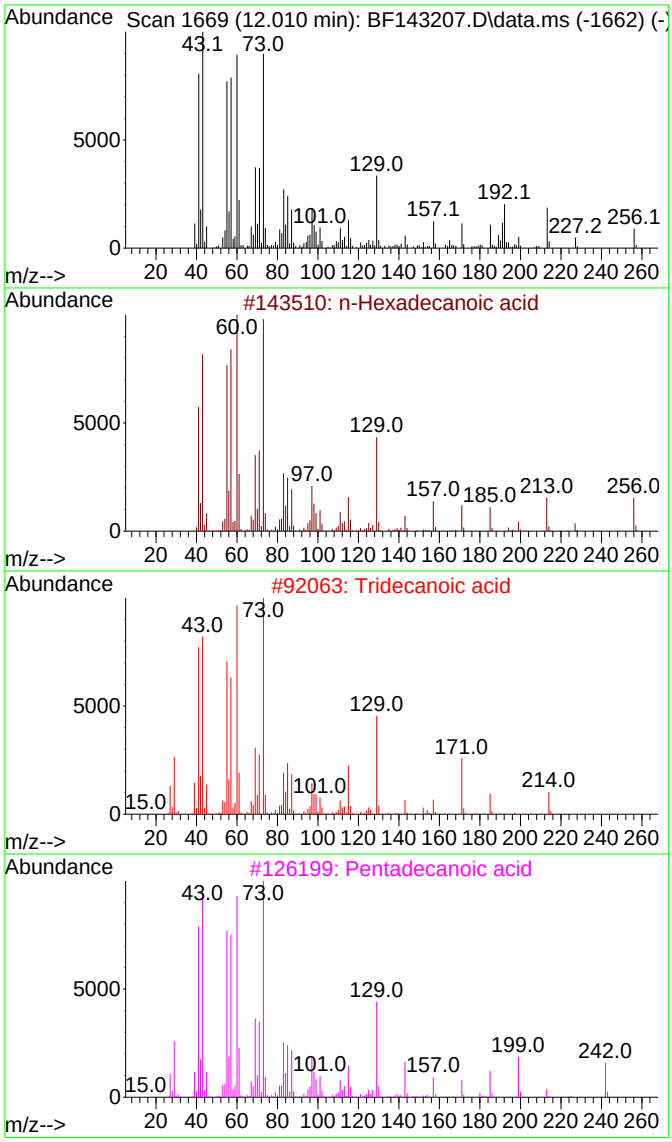
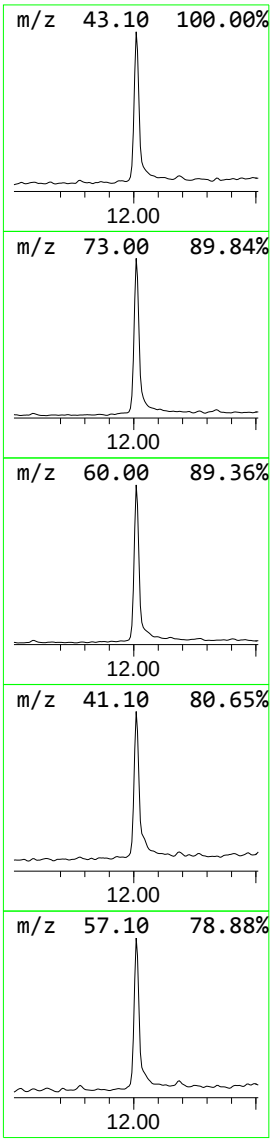
Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.010	12.80 ng	497472	Phenanthrene-d10	11.492

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	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Undecanoic acid	186	C11H22O2	000112-37-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60





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Operator : RC/JU
Sample : Q2649-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

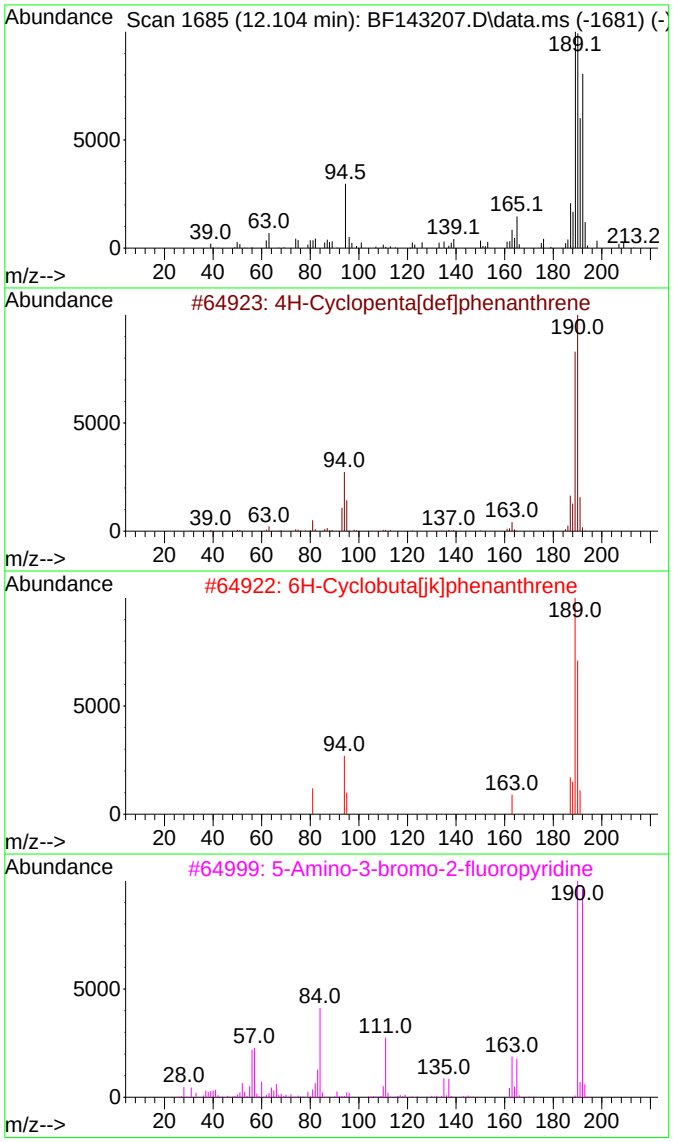
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

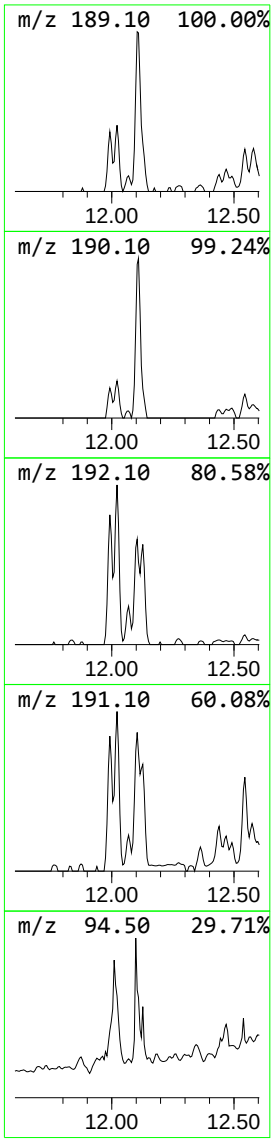
****

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.104	2.28 ng	88485	Phenanthrene-d10	11.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	52
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	49
3	5-Amino-3-bromo-2-fluoropyridine	190	C5H4BrFN2	209328-99-4	35
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	35
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	30





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Operator : RC/JU
Sample : Q2649-01
Misc :
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Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

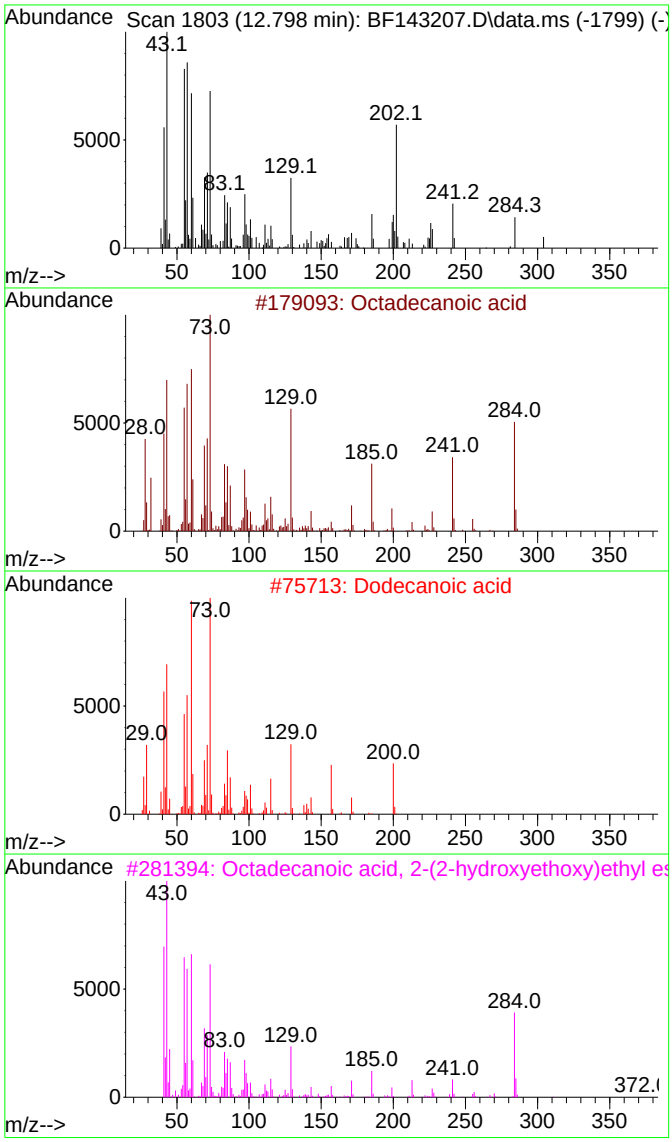
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

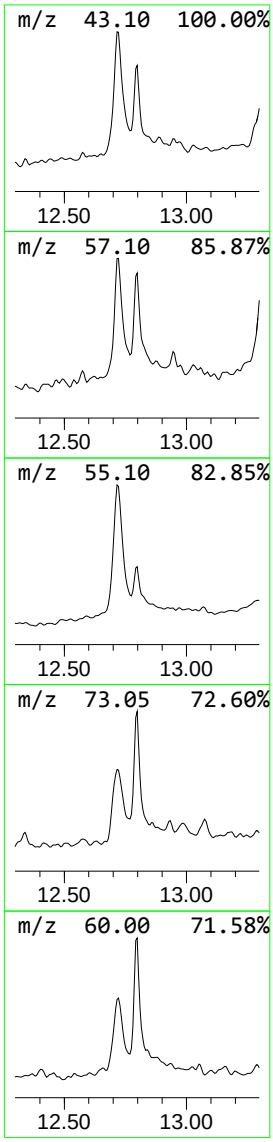
****

Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.798	2.59 ng	100502	Phenanthrene-d10	11.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	Dodecanoic acid	200	C12H24O2	000143-07-7	55
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	49
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	46
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	43





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Data File : BF143207.D
Acq On : 23 Jul 2025 00:12
Operator : RC/JU
Sample : Q2649-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

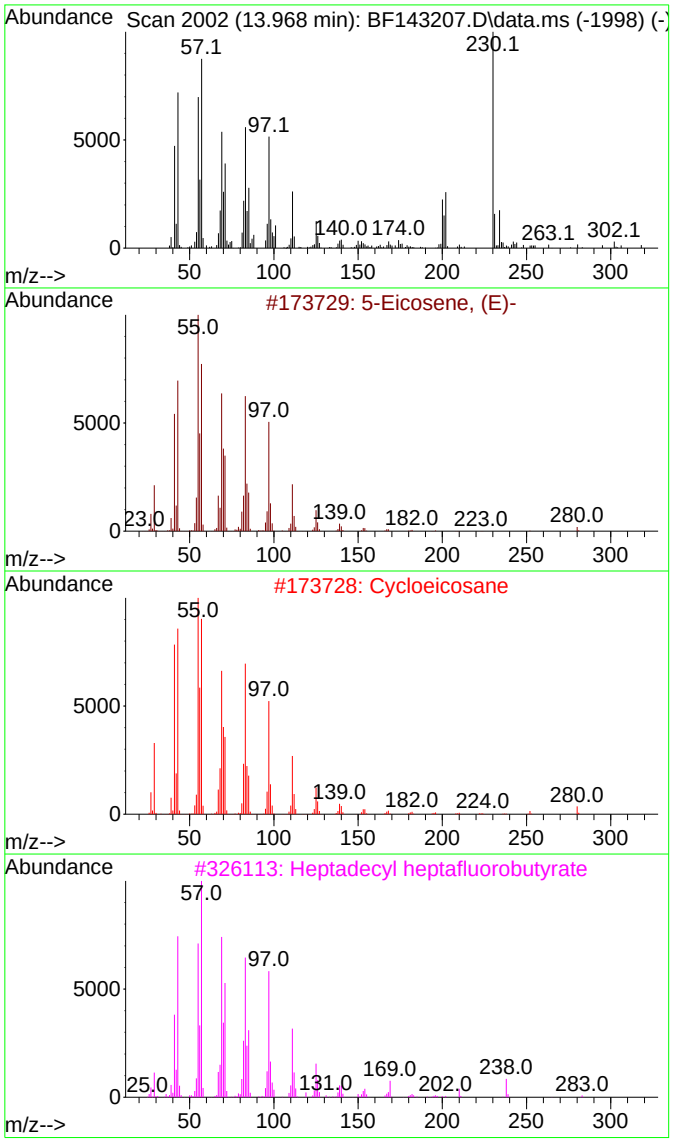
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

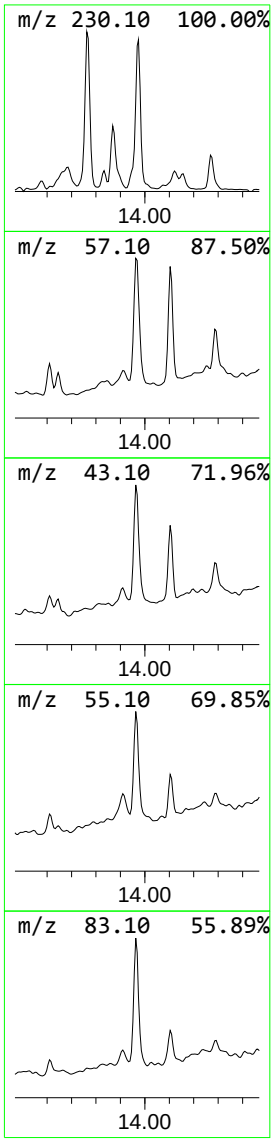
****

Peak Number 7 5-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.968	3.49 ng	253091	Chrysene-d12	14.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	95
2	Cycloeicosane	280	C20H40	000296-56-0	64
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	64
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	64
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	50





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BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

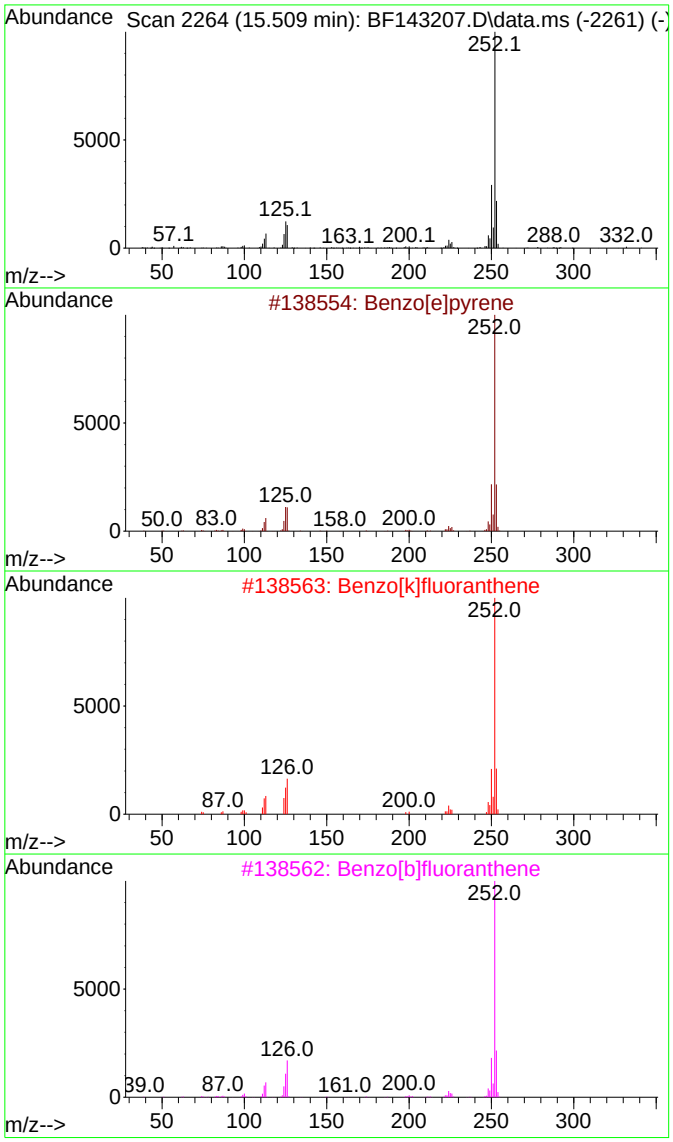
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

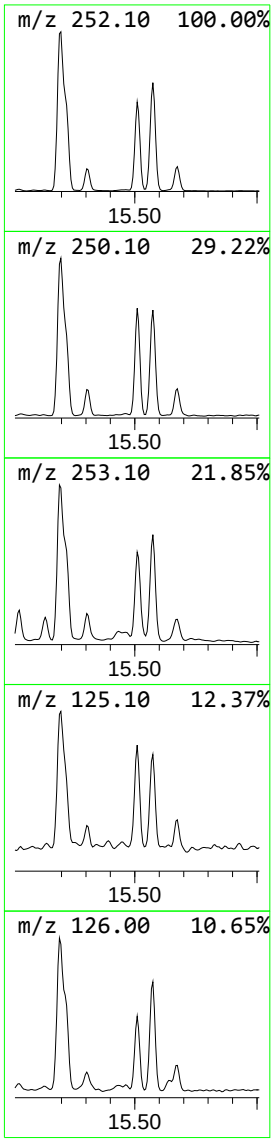
****

Peak Number 8 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.509	4.69 ng	156582	Perylene-d12	15.639

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
4	Benzo[a]pyrene	252	C20H12	000050-32-8	96
5	Perylene	252	C20H12	000198-55-0	95





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072225\
Data File : BF143207.D
Acq On : 23 Jul 2025 00:12
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Sample : Q2649-01
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ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.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...	2.304	25.1	ng	788929	1	6.969	628576	20.0
2-Pentanone, 4-...	5.198	6.6	ng	207421	1	6.969	628576	20.0
Benzophenone	10.710	5.9	ng	213790	3	10.004	726049	20.0
n-Hexadecanoic ...	12.010	12.8	ng	497472	4	11.492	777512	20.0
4H-Cyclopenta[d...	12.104	2.3	ng	88485	4	11.492	777512	20.0
Octadecanoic acid	12.798	2.6	ng	100502	4	11.492	777512	20.0
5-Eicosene, (E)-	13.968	3.5	ng	253091	5	14.133	1449480	20.0
Benzo[e]pyrene	15.509	4.7	ng	156582	6	15.639	667031	20.0